10/ 501,033

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NEWS 5	DEC 14	2006 MeSH terms loaded for MEDLINE file segment of TOXCENTER
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NEWS 7	DEC 21	IPC search and display fields enhanced in CA/CAplus with the IPC reform
NEWS 8	DEC 23	New IPC8 SEARCH, DISPLAY, and SELECT fields in USPATFULL/ USPAT2
NEWS 9	JAN 13	IPC 8 searching in IFIPAT, IFIUDB, and IFICDB
NEWS 10	JAN 13	New IPC 8 SEARCH, DISPLAY, and SELECT enhancements added to INPADOC
NEWS 11	JAN 17	Pre-1988 INPI data added to MARPAT
NEWS 12	JAN 17	IPC 8 in the WPI family of databases including WPIFV
NEWS 13	JAN 30	Saved answer limit increased
NEWS 14	JAN 31	Monthly current-awareness alert (SDI) frequency added to TULSA
NEWS 15	FEB 21	STN AnaVist, Version 1.1, lets you share your STN AnaVist visualization results
NEWS 16	FEB 22	Status of current WO (PCT) information on STN
NEWS 17	FEB 22	The IPC thesaurus added to additional patent databases on STN
NEWS 18	FEB 22	Updates in EPFULL; IPC 8 enhancements added
NEWS 19	FEB 27	New STN AnaVist pricing effective March 1, 2006
NEWS 20	FEB 28	MEDLINE/LMEDLINE reload improves functionality
NEWS 21	FEB 28	TOXCENTER reloaded with enhancements
NEWS 22	FEB 28	REGISTRY/ZREGISTRY enhanced with more experimental spectral property data
NEWS 23	MAR 01	INSPEC reloaded and enhanced
NEWS 24	MAR 03	Updates in PATDPA; addition of IPC 8 data without attributes

NEWS EXPRESS FEBRUARY 15 CURRENT VERSION FOR WINDOWS IS V8.01a,
CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
AND CURRENT DISCOVER FILE IS DATED 19 DECEMBER 2005.
V8.0 AND V8.01 USERS CAN OBTAIN THE UPGRADE TO V8.01a AT
http://download.cas.org/express/v8.0-Discover/

NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS INTER	General Internet Information
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* * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 17:18:03 ON 07 MAR 2006

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 17:18:13 ON 07 MAR 2006
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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 6 MAR 2006 HIGHEST RN 876011-49-3
DICTIONARY FILE UPDATES: 6 MAR 2006 HIGHEST RN 876011-49-3

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TSCA INFORMATION NOW CURRENT THROUGH January 6, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

****
* *
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, *
* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *
* *
****

Structure search iteration limits have been increased. See HELP SLIMITS for details.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

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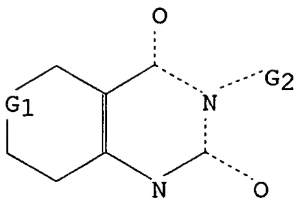
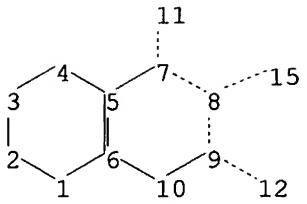
Uploading C:\Program Files\Stnexp\Queries\10501033.str





chain nodes :
11 12 15
ring nodes :
1 2 3 4 5 6 7 8 9 10
chain bonds :
7-11 8-15 9-12
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10
exact/norm bonds :
5-6 5-7 6-10 7-8 7-11 8-9 8-15 9-10 9-12
exact bonds :
1-2 1-6 2-3 3-4 4-5
isolated ring systems :
containing 1 :

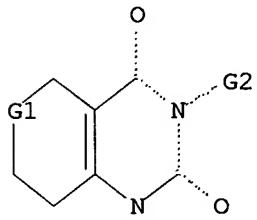
G1:O,S,CH2

G2:C,H,O

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:CLASS 12:CLASS 15:CLASS

L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR



G1 O,S,CH2

G2 C,H,O

Structure attributes must be viewed using STN Express query preparation.

=> s l1 sample
SAMPLE SEARCH INITIATED 17:18:37 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 2286 TO ITERATE

10/ 501,033

87.5% PROCESSED 2000 ITERATIONS 22 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 42853 TO 48587
PROJECTED ANSWERS: 202 TO 802

L2 22 SEA SSS SAM L1

=> s l1 full
FULL SEARCH INITIATED 17:18:45 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 44339 TO ITERATE

100.0% PROCESSED 44339 ITERATIONS 475 ANSWERS
SEARCH TIME: 00.00.01

L3 475 SEA SSS FUL L1

=> file hcaplus
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 166.94 167.15

FILE 'HCAPLUS' ENTERED AT 17:18:53 ON 07 MAR 2006
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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FILE COVERS 1907 - 7 Mar 2006 VOL 144 ISS 11
FILE LAST UPDATED: 6 Mar 2006 (20060306/ED)

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This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d his

(FILE 'HOME' ENTERED AT 17:18:03 ON 07 MAR 2006)

FILE 'REGISTRY' ENTERED AT 17:18:13 ON 07 MAR 2006
L1 STRUCTURE UPLOADED
L2 22 S L1 SAMPLE
L3 475 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 17:18:53 ON 07 MAR 2006

=> s l3

10/ 501,033

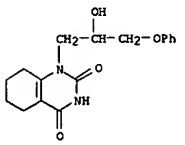
L4 87 L3

=> d l4 1- ibib abs fhitstr
YOU HAVE REQUESTED DATA FROM 87 ANSWERS - CONTINUE? Y/(N):y

L4 ANSWER 1 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2005:316578 HCAPLUS
DOCUMENT NUMBER: 143:7675
TITLE: Synthesis and rearrangement of cycloalkyl[1,2-e]oxazolo[3,2-a]pyrimidin-8/9-ones: an access to cycloalkyl[1,2-d]oxazolo[3,2-a]pyrimidin-5-ones
AUTHOR(S): Adetchessi, Ouro-Sama; Leger, Jean-Michel; Guillon, Jean; Forfar-Bares, Isabelle; Bosc, Jean-Jacques; Jarry, Christian
CORPORATE SOURCE: UFR de Pharmacie, EA 2962--Pharmacochimie, Universite Victor Segalen Bordeaux 2, Bordeaux, 33076, Fr.
SOURCE: Tetrahedron (2005), 61(18), 4453-4460
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 143:7675

AB 2-Substituted-4a-hydroxy-9H-cycloalka[1,2-e]oxazolo[3,2-a]pyrimidin-9-ones were synthesized by a one-step cyclocondensation from the 5-substituted-2-amino-2-oxazolines with Et 2-oxocyclohexanecarboxylate in ethanol at room temperature, and easily dehydrated to provide 2-substituted-9H-cycloalka[1,2-e]oxazolo[3,2-a]pyrimidin-9-ones. In refluxing xylene, the reaction conducted with various Et 2-oxocycloalkanecarboxylates led to the two isomeric 2-substituted-8/9H-cycloalka[1,2-e]oxazolo[3,2-a]pyrimidin-8/9-ones and 2-substituted-5H-cycloalka[1,2-d]oxazolo[3,2-a]pyrimidin-5-ones. The structure of some compds. was unambiguously established using X-ray crystallog. According to results from the DSC anal. of compound , formation of the thermodynamically stable pyrimidinones could be related to an intramol. rearrangement of kinetically controlled pyrimidinones.

IT 852571-52-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation by ring cleavage of oxazolopyrimidinones)
RN 852571-52-9 HCAPLUS
CN 2,4(1H,3H)-Quinazolinedione, 5,6,7,8-tetrahydro-1-(2-hydroxy-3-phenoxypropyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

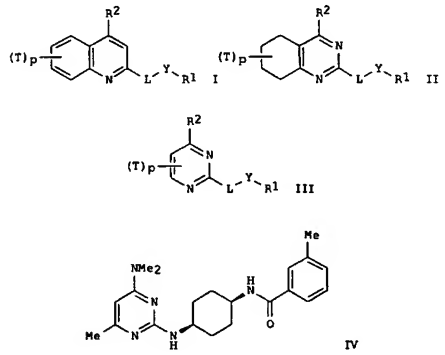
L4 ANSWER 2 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:875032 HCAPLUS
DOCUMENT NUMBER: 141:350191
TITLE: Preparation of quinoline, tetrahydroquinazoline, and pyrimidine derivatives as MCH antagonist for treatment of CNS disorders
INVENTOR(S): Sekiguchi, Yoshinori; Kanuma, Kosuke; Omodera, Katsunori; Busujima, Tsuyoshi; Tran, Thuy-Anh; Han, Sangdon; Casper, Martin; Kramer, Bryan A.; Semple, Graeme; Zou, Ning
PATENT ASSIGNEE(S): Taisho Pharmaceutical Co. Ltd., Japan
SOURCE: Eur. Pat. Appl., 586 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1464335	A2	20041006	EP 2004-7651	20040330
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK				
EP 1464335	A2	20041006	EP 2004-7651	20040330
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK				

PRIORITY APPLN. INFO.:
US 2003-458530P P 20030331
US 2003-495911P P 20030819
US 2003-510186P P 20031009
US 2003-530360P P 20031216
EP 2004-7651 A 20040330

GI

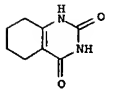
L4 ANSWER 2 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



AB Title compds. I, II, and III [wherein R1 = (un)substituted (cyclo)alkyl, (cyclo)alkenyl, alkynyl, aryl; R2 = H, halo, OH, carboxy, carbamoyl, amino, (un)substituted alkyl, alkoxy; T = independently H, halo, OH, carboxy, carbamoyl, amino, cyano, NO2, alkenyl, alkynyl, cycloalkyl, (un)substituted alkyl, alkoxy; p = 0-5; L = aminocycloalkylideneamino, etc.; Y = bond, CH2, CO2, OCO, SO2, CO, CS, CONH, CSNH, etc.; with provisos; and pharmaceutically acceptable salts, hydrates, or solvates thereof] were prepared as antagonists of melanin concentrating hormone (MCH), an endogenous ligand of G-protein coupled receptors (GPCRs). Examples include solution and solid phase general synthetic methods and phys. data for nearly 3400 invention compds. In addition, all exemplified compds. were assayed using high throughput functional screening to detect intracellular Ca2+ concns. for accessing GPCR activation. For instance, reaction of 2,4-dichloro-6-methylpyrimidine with dimethylamine gave 2-chloro-4-(dimethylamino)-6-methylpyrimidine (40%), which was coupled with cis-(4-aminocyclohexyl)carbamic acid tert-Bu ester (60%). Deprotection (72%), amidation, and workup provided the benzamide IV•TFA. The latter demonstrated MCH antagonist activity with an IC50 value of 7.6 nM. Thus, pharmaceutical compns. comprising I are useful for the prophylaxis or treatment of improving memory function, sleeping and arousal, anxiety, depression, mood disorders, seizure, obesity, diabetes, appetite and eating disorders, cardiovascular disease, hypertension, dyslipidemia, myocardial infarction, binge eating disorders including bulimia, anorexia, mental disorders including manic depression, schizophrenia, delirium, dementia, stress, cognitive disorders, attention deficit disorder, substance abuse disorders, and dyskinesias including Parkinson's disease, epilepsy, and addiction (no data). This is part II of three in a series covering the patent.

IT 35042-48-9P, 5,6,7,8-Tetrahydroquinazoline-2,4-diol

L4 ANSWER 2 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; prepn. of quinolines, quinazolines, and pyrimidines as MCH antagonist for treatment of CNS disorders)
RN 35042-48-9 HCAPLUS
CN 2,4(1H,3H)-Quinazolinedione, 5,6,7,8-tetrahydro- (9CI) (CA INDEX NAME)

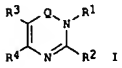


L4 ANSWER 3 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:857326 HCAPLUS
DOCUMENT NUMBER: 141:309639
TITLE: Dipeptidyl peptidase inhibitors
INVENTOR(S): Feng, Jun; Gwaltney, Stephen L.; Kaldor, Stephen W.; Stafford, Jeffrey A.; Wallace, Michael B.; Zhang, Zhiyuan
PATENT ASSIGNEE(S): Syrrx, Inc., USA
SOURCE: PCT Int. Appl., 244 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004087053	A2	20041014	WO 2004-US9217	20040324
WO 2004087053	C2	20041111		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2518465	AA	20041014	CA 2004-2518465	20040324
US 2004242568	A1	20041202	US 2004-809636	20040324
US 2004242566	A1	20041202	US 2004-809638	20040324
US 2004259870	A1	20041223	US 2004-809637	20040324
US 2005004117	A1	20050106	US 2004-809635	20040324
EP 1608317	A2	20051228	EP 2004-758366	20040324
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK				

PRIORITY APPLN. INFO.: US 2003-457785P P 20030325
WO 2004-US9217 W 20040324

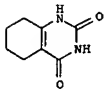
OTHER SOURCE(S): MARPAT 141:309639
GI



I

AB Dipeptidyl peptidase IV inhibitors I [Q = CO, SO, SO2, C:NR5; R1 = ZR6; Z = moiety providing 1-6 atom separation between R6 and ring; R2 = (substituted)3-7-membered ring; R3,R4 = taken together form a (substituted)5-6-membered ring; R5 = H, (substituted)alkyl, cycloalkyl, etc.; R6 = (substituted)C3-7-cycloalkyl or aryl] are disclosed. Thus, 2-[2-(3-aminopiperidin-1-yl)-6,7-dimethoxy-4-oxo-4H-quinazolin-3-

L4 ANSWER 3 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
ylmethyl]benzonitrile (I; R1 = 2-cyanophenylmethyl; R2 = 3-aminopiperidin-1-yl; R3,R4 = dimethoxyphenyl) was synthesized. This compd. exhibited enhanced stability in rat liver microsomes.
IT 35042-48-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(dipeptidyl peptidase inhibitors)
RN 35042-48-9 HCAPLUS
CN 2,4(1H,3H)-Quinazolinedione, 5,6,7,8-tetrahydro- (9CI) (CA INDEX NAME)



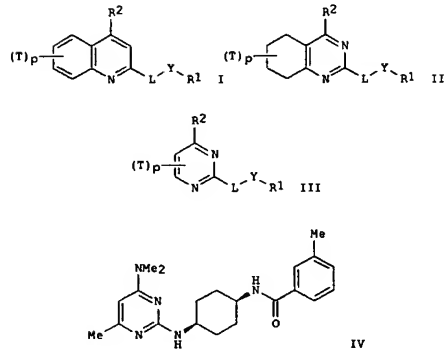
L4 ANSWER 4 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:822842 HCAPLUS
DOCUMENT NUMBER: 141:314346
TITLE: Preparation of quinoline, tetrahydroquinazoline, and pyrimidine derivatives as MCH antagonist for treatment of CNS disorders
INVENTOR(S): Sekiguchi, Yoshinori; Kanuma, Kosuke; Omodera, Katsunori; Busujima, Tsuyoshi; Tran, Thuy-Anh; Han, Sangdon; Casper, Martin; Kramer, Bryan A.; Semple, Graeme; Zou, Ning
PATENT ASSIGNEE(S): Taisho Pharmaceutical Co. Ltd., Japan; Arena Pharmaceuticals, Inc.
SOURCE: Eur. Pat. Appl., 586 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1464335	A2	20041006	EP 2004-7651	20040330
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK				
US 2005197350	A1	20050908	US 2004-812075	20040330
CA 2518913	AA	20041014	CA 2004-2518913	20040331
WO 2004087669	A1	20041014	WO 2004-JP4624	20040331
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
JP 2004300156	A2	20041028	JP 2004-107965	20040331
NO 2005004999	A	20051107	NO 2005-4999	20051027

PRIORITY APPLN. INFO.: US 2003-458530P P 20030331
US 2003-495911P P 20030819
US 2003-510186P P 20031009
US 2003-530360P P 20031216
WO 2004-JP4624 W 20040331

OTHER SOURCE(S): MARPAT 141:314346
GI

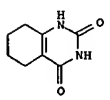
L4 ANSWER 4 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



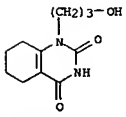
I II III IV

AB Title compds. I, II, and III [wherein R1 = (un)substituted (cyclo)alkyl, (cyclo)alkenyl, alkynyl, aryl; R2 = H, halo, OH, carboxy, carbamoyl, amino, (un)substituted alkyl, alkoxy; T = independently H, halo, OH, carboxy, carbamoyl, amino, cyano, NO2, alkenyl, alkynyl, cycloalkyl, (un)substituted alkyl, alkoxy; p = 0-5; L = aminocycloalkylideneamino, etc.; Y = bond, CH2, CO2, OCO, SO2, CO, CS, CONH, CSNH, etc.; with provisos; and pharmaceutically acceptable salts, hydrates, or solvates thereof] were prepared as antagonists of melanin concentrating hormone (MCH), an endogenous ligand of G-protein coupled receptors (GPCRs). Examples include solution and solid phase general synthetic methods and phys. data for nearly 3400 invention compds. In addition, all exemplified compds. were assayed using high throughput functional screening to detect intracellular Ca2+ concns. for accessing GPCR activation. For instance, reaction of 2,4-dichloro-6-methylpyrimidine with dimethylamine gave 2-chloro-4-(dimethylamino)-6-methylpyrimidine (40%), which was coupled with cis-(4-aminocyclohexyl)carbamic acid tert-Bu ester (60%). Deprotection (72%), amidation, and workup provided the benzamide IV•TFA. The latter demonstrated MCH antagonist activity with an IC50 value of 7.6 nM. Thus, pharmaceutical compns. comprising I are useful for the prophylaxis or treatment of improving memory function, sleeping and arousal, anxiety, depression, mood disorders, seizure, obesity, diabetes, appetite and eating disorders, cardiovascular disease, hypertension, dyslipidemia, myocardial infarction, binge eating disorders including bulimia, anorexia, mental disorders including manic depression, schizophrenia, delirium, dementia, stress, cognitive disorders, attention deficit disorder, substance abuse disorders, and dyskinesias including Parkinson's disease, epilepsy, and addiction (no data). This is part I of three in a series covering the patent.
IT 35042-48-9P, 5,6,7,8-Tetrahydroquinazoline-2,4-diol

L4 ANSWER 4 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; prepn. of quinolines, quinazolines, and pyrimidines as MCH antagonist for treatment of CNS disorders)
RN 35042-48-9 HCAPLUS
CN 2,4(1H,3H)-Quinazolinedione, 5,6,7,8-tetrahydro- (9CI) (CA INDEX NAME)



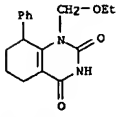
L4 ANSWER 5 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
RN 72458-91-4 HCAPLUS
CN 2,4(1H,3H)-Quinazolinedione, 5,6,7,8-tetrahydro-1-(3-hydroxypropyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 5 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:115765 HCAPLUS
DOCUMENT NUMBER: 140:368067
TITLE: A study of the influence of newly synthesized acyclonucleosides and 1,2,3,4-tetrahydroisoquinoline derivatives on deoxythymidine and deoxycytidine kinase activities in human neurofibrosarcoma and ovarian cancer
AUTHOR(S): Modrzejewska, Hanna; Brzezinska, Elzbieta; Draminski, Marcin; Zgit-Wroblewska, Anna; Krzykowska, Katarzyna; Rozponczyk, Elzbieta; Greger, Janusz
CORPORATE SOURCE: Department of Medical Biochemistry, Institute of Physiology and Biochemistry, Medical University of Lodz, Lodz, Pol.
SOURCE: Acta Biochimica Polonica (2003), 50(4), 1175-1185
CODEN: ABPLAF; ISSN: 0001-527X
PUBLISHER: Polish Biochemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 140:368067
AB The influence of nine newly synthesized uracil acyclonucleosides, and 36 derivs. of 1,2,3,4-tetrahydroisoquinoline on the activity of enzymes catalyzing dTMP and dGMP synthesis, on the content of dTTP and dGTP in acid soluble fraction and on the incorporation of [14C]dThd and [14C]dGuo into DNA in tumor homogenates was studied. The influence of the compds. was studied in the cytosol from intraoperatively excised human tumors - neurofibrosarcoma and ovarian cancer. It was shown that dTMP and dGMP synthesis is inhibited competitively by 34.1±4.0% in both types of tumors by 0.2 mM 1-N-(3'-hydroxypropyl)-6-methyluracil (1) and 0.2 mM 1-N-(3'-hydroxypropyl)-5,6- tetramethyleneuracil (2). The mentioned acyclonucleosides reduced the content of dTTP and dGTP in the acid soluble fraction of tumors (59.7±3.1% of control). 1-(4-Chlorophenyl)-6,7-dihydroxy-1,2,3,4-tetrahydroisoquinoline (3), 1-(2,3-dichlorophenyl)-6,7-dihydroxy 1,2,3,4-tetrahydroisoquinoline (4) and 1-(3-methoxyphenyl)-6,7-dihydroxy 1,2,3,4-tetrahydroisoquinoline (5) at 0.2 mM concentration caused a mixed type inhibition of the synthesis of dTMP and dGMP by, on average, 33.2±4.4%, and reduced the content of dTTP and dGTP in the acid soluble fraction (52.6±3.7% of control) but were active only in the cytosol of neurofibrosarcoma. While acyclonucleosides undergo Phosphorylation in the cytosol by cellular kinases, with their triphosphates being active acyclonucleoside metabolites, active 1,3,4,5-tetrahydroisoquinoline derivs. (compds. not containing a deoxyribose moiety), cannot be phosphorylated. ACN and THI derivs. which inhibit dThd and dCyd kinase activities, inhibit also the incorporation of [14C]dThd and [14C]dGuo (ACN - 50.2±2.7%, THI - 53.4±3.9% of incorporation inhibition) into tumor DNA. The obtained results point to the mechanism of uracil acyclonucleosides and 1,2,3,4-tetrahydroisoquinoline biol. activity consisting in inhibiting the synthesis of DNA components.
IT 72458-91-4P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation, structure-activity relationship and antitumor effect of acyclonucleosides and 1,2,3,4-tetrahydroisoquinoline derivs. on deoxythymidine and deoxycytidine kinase activities in human neurofibrosarcoma and ovarian cancer)

L4 ANSWER 6 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:605969 HCAPLUS
DOCUMENT NUMBER: 140:27794
TITLE: Multiple pathways in the synthesis of new annelated analogues of 6-benzyl-1-(ethoxymethyl)-5-isopropyluracil (emivirine)
AUTHOR(S): Therkelsen, Frans D.; Hansen, Anne-Lene L.; Pedersen, Erik B.; Nielsen, Claus
CORPORATE SOURCE: Nucleic Acid Center, Department of Chemistry, University of Southern Denmark, Odense, DK-5230, Den.
SOURCE: Organic & Biomolecular Chemistry (2003), 1(16), 2908-2918
CODEN: OBCRAK; ISSN: 1477-0520
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 140:27794
AB Condensation of 3-(3,5-dimethylphenyl)-2-oxocyclopentanecarboxamide (11) with oxalyl chloride and condensation of Et 2-benzylamino-5-methyl-3-phenylcyclopent-1-enecarboxylate (17a) with trimethylsilyl isothiocyanate gave 7-(3,5-dimethylphenyl)-6,7-dihydro-5H-cyclopenta[e][1,3]oxazine-2,4-dione (I) and 1-benzyl-5-methyl-7-phenyl-2-thioxo-1,2,3,5,6,7-hexahydrocyclopentapyrimidin-4-one (II), resp. Acid catalyzed ring-closure of 6-(4-methyl-1-phenylpent-3-enyl)-2-thioxo-2,3-dihydro-1H-pyrimidin-4-one (26) and radical mediated ring-closure of 1,3-bis(benzyloxymethyl)-5-bromo-6-(1-phenylbut-3-enyl)-1H-pyrimidine-2,4-dione (32a) gave 5,5-dimethyl-8-phenyl-5,6,7,8-tetrahydro-1H-quinazoline-2,4-dione (III) and 1,3-bis(benzyloxymethyl)-5-methyl-7-phenyl-1,5,6,7-tetrahydrocyclopentapyrimidine-2,4-dione (IV), resp. Annelated emivirine analogs 7-(3,5-dimethylphenyl)-1-ethoxymethyl-1,5,6,7-tetrahydrocyclopentapyrimidine-2,4-dione (V), 1-ethoxymethyl-5,5-dimethyl-8-phenyl-5,6,7,8-tetrahydro-1H-quinazoline-2,4-dione (VI), and 1-ethoxymethyl-5-methyl-7-phenyl-1,5,6,7-tetrahydrocyclopentapyrimidine-2,4-dione (VII) were obtained in few steps from I-IV. These new analogs can be considered as conformationally locked analogs of emivirine. However, V-VII showed lower activities against HIV-1 than emivirine and it is concluded that the locked conformation disfavors activity against HIV-1.
IT 312312-69-9
RL: PAC (Pharmacological activity); BIOL (Biological study)
(preparation and anti HIV-1 activity of conformationally locked analogs of emivirine)
RN 312312-69-9 HCAPLUS
CN 2,4(1H,3H)-Quinazolinedione, 1-(ethoxymethyl)-5,6,7,8-tetrahydro-8-phenyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 6 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

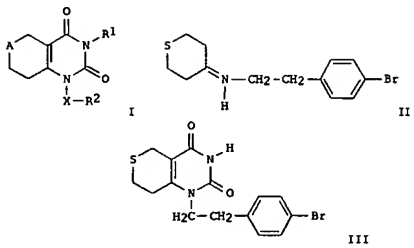
L4 ANSWER 7 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2003:570967 HCAPLUS
DOCUMENT NUMBER: 139:117436
TITLE: Preparation of tetrahydroquinazolinediones and related compds. as poly(adenosine diphosphoribose) synthetase inhibitors for the treatment of ischemia and reperfusion injury
INVENTOR(S): Albrecht, Barbara; Gerisch, Michael; Haerter, Michael; Krahn, Thomas; Oehme, Felix; Schlemmer, Karl-Heinz; Steinhagen, Henning
PATENT ASSIGNEE(S): Bayer Aktiengesellschaft, Germany
SOURCE: PCT Int. Appl., 74 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003059892	A1	20030724	WO 2003-EP27	20030103
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
DE 10201240	A1	20030724	DE 2002-10201240	20020115
CA 2473362	AA	20030724	CA 2003-2473362	20030103
AU 2003206694	A1	20030730	AU 2003-206694	20030103
EP 1467975	A1	20041020	EP 2003-704354	20030103
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
US 2005159431	A1	20050721	US 2003-501033	20030103
PRIORITY APPLN. INFO.:			DE 2002-10201240 A	20020115
			WO 2003-EP27 W	20030103

OTHER SOURCE(S): MARPAT 139:117436
GI

L4 ANSWER 7 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



I II

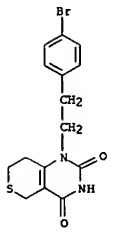
III

AB Title compds. I [A = CH2, O, S; X = alkandiyl (sic), where a methylene group can be replaced by an oxygen; R1 = H, alkoxycarbonyl; R2 = (un)substituted aryl, heteroaryl, e.g, NO2, halo, CN, etc.] and their pharmaceutically acceptable salts and formulations were prepared For example, condensation of imine II, prepared in situ from 2-(4-bromophenyl)ethylamine and tetrahydro-4H-thiopyran-4-one, and chlorocarbonylisocyanate, afforded tetrahydroquinazolinedione III in 74% yield. In poly(adenosine diphosphoribose) synthetase inhibition assays, 7-examples of compds. I exhibited IC50 values ranging from 20-800 nM, e.g., the IC50 value of tetrahydroquinazolinedione III was 60 nM. Compds. I are claimed useful for the treatment of ischemia and reperfusion injury.

IT 564480-38-2P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(drug candidate; preparation of tetrahydroquinazolinediones and related compds. as poly(ADP ribose) synthetase inhibitors for the treatment of ischemia and reperfusion injury)

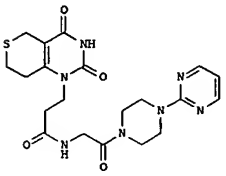
RN 564480-38-2 HCAPLUS
CN 2H-Thiopyrano[4,3-d]pyrimidine-2,4(3H)-dione, 1-[2-(4-bromophenyl)ethyl]-1,5,7,8-tetrahydro- (9CI) (CA INDEX NAME)

L4 ANSWER 7 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 8 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:767295 HCAPLUS
DOCUMENT NUMBER: 138:137076
TITLE: Substituted uracil derivatives as potent inhibitors of poly(ADP-ribose)polymerase-1 (PARP-1)
AUTHOR(S): Steinhagen, Henning; Gerisch, Michael; Mittendorf, Joachim; Schlemmer, Karl-Heinz; Albrecht, Barbara
CORPORATE SOURCE: Institute of Medicinal Chemistry, Pharma Research Centre, Bayer AG, Wuppertal, D-42096, Germany
SOURCE: Bioorganic & Medicinal Chemistry Letters (2002), 12(21), 3187-3190
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:137076
GI



I

AB A new class of PARP-1 inhibitors, namely substituted fused uracil derivs. such as I, were synthesized. Starting from a derivative with an IC50=2 μM the chemical optimization program led to compds. with more than a 100-fold increase in potency (IC50<20 nM). Addnl., physicochem. and pharmacokinetic properties were evaluated. It could be shown that compds. bearing a piperazine or Ph substituted βAla-Gly side chain exhibited the best overall profile.

IT 425635-00-3P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(preparation of uracil derivs. as inhibitors of poly(ADP-ribose)polymerase-1)

RN 425635-00-3 HCAPLUS
CN 2H-Thiopyrano[4,3-d]pyrimidine-1(5H)-propanamide, N-[2-(4-bromophenyl)-2-oxoethyl]-3,4,7,8-tetrahydro-2,4-dioxo- (9CI) (CA INDEX NAME)

L4 ANSWER 8 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

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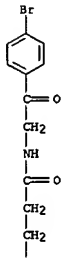
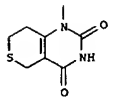


PAGE 2-A

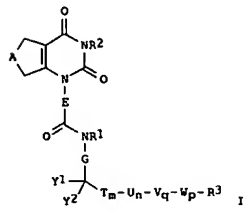


REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 9 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:366971 HCAPLUS
DOCUMENT NUMBER: 136:386124
TITLE: Preparation of amidoalkyluracils as inhibitors of poly(ADP-ribose)synthetase (PARS)
INVENTOR(S): Albrecht, Barbara; Gerisch, Michael; Handke, Gabriele; Jensen, Axel; Krahn, Thomas; Nickl, Werner; Oehme, Felix; Schlemmer, Karl-Heinz; Steinhagen, Henning
PATENT ASSIGNEE(S): Bayer Ag, Germany
SOURCE: Ger. Offen., 70 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 10056312	A1	20020516	DE 2000-10056312	20001114
CA 2428335	AA	20020523	CA 2001-2428335	20011102
WO 2002040455	A1	20020523	WO 2001-EP12694	20011102
WO 2002040455	C1	20020718		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2002024825	A5	20020527	AU 2002-24825	20011102
EP 1339699	A1	20030903	EP 2001-994632	20011102
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
US 2005075347	A1	20050407	US 2003-416622	20031229
PRIORITY APPLN. INFO.:			DE 2000-10056312 A	20001114
			WO 2001-EP12694 W	20011102

OTHER SOURCE(S): MARPAT 136:386124
GI



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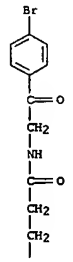
L4 ANSWER 9 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

AB Title compds. [I; A = O, CH2D, DCH2, CH:CHCH2, CH2CH:CH, CH2CH2D, DCH2CH2, CH2DCH2; D = CH2, O, S; E, G = (substituted) alkylene, cycloalkylene; T = CH2; U, V = (substituted) aryl, heterocyclyl; W = O, S, CO2, OCO, NR4; R4 = H, alkyl; m, n, q, p = 0, 1; X = O, S, NR5; R5 = H, alkyl, PhCH2; Y1 = H; Y2 = OH; Y1Y2 = O, S, NR6; R6 = H, alkyl, PhCH2; R1 = H, alkyl, (halo)cycloalkyl; R2 = H, alkoxycarbonyl; R3 = (substituted) aryl, heterocyclyl] were prepared Thus, a mixture of 3-(2,4-dioxo-3,4,5,6,7,8-hexahydro-1(2H)-quinazolinyl)propanoic acid (preparation given) and 2-(2-naphthyl)-2-oxo-1-ethanamine hydrochloride in CH2Cl2 was treated with diisopropylamine and 4-dimethylaminopyridine, followed by addition of 1,3-dicyclohexylcarbodiimide at 0° and stirring for 18 h at room temperature, to give 48% 3-(2,4-dioxo-3,4,5,6,7,8-hexahydro-1(2H)-quinazolinyl)-N-[2-(2-naphthyl)-2-oxo-1-ethyl]propanamide. Several I inhibited PARS with IC50 = 8.5-80 nM.

IT 425635-00-3P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of amidoalkyluracils as inhibitors of poly(ADP-ribose)synthetase (PARS))

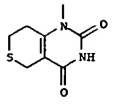
RN 425635-00-3 HCAPLUS
CN 2H-Thiopyrano[4,3-d]pyrimidine-1(5H)-propanamide, N-[2-(4-bromophenyl)-2-oxoethyl]-3,4,7,8-tetrahydro-2,4-dioxo- (9CI) (CA INDEX NAME)

PAGE 1-A



L4 ANSWER 9 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 2-A

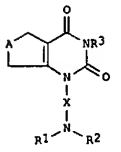


L4 ANSWER 10 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2002:72062 HCAPLUS
DOCUMENT NUMBER: 136:134774
TITLE: Preparation of fused amidoalkyluracils as poly(ADP-ribose) synthetase inhibitors
INVENTOR(S): Haerter, Michael; Albrecht, Barbara; Gerisch, Michael; Handke, Gabriele; Huetter, Joachim; Jensen, Axel; Krahn, Thomas; Mittendorf, Joachim; Oehme, Felix; Schlemmer, Karl-Heinz; Steinhagen, Henning
PATENT ASSIGNEE(S): Bayer Aktiengesellschaft, Germany
SOURCE: PCT Int. Appl., 113 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002006247	A1	20020124	WO 2001-EP7670	20010705
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
DE 10034801	A1	20020131	DE 2000-10034801	20000718
CA 2416036	AA	20020124	CA 2001-2416036	20010705
EP 1303497	A1	20030423	EP 2001-947443	20010705
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
US 2003022905	A1	20030130	US 2001-906296	20010716
US 6649618	B2	20031118		
PRIORITY APPLN. INFO.:			DE 2000-10034801	A 20000718
			WO 2001-EP7670	W 20010705

OTHER SOURCE(S): MARPAT 136:134774
GI



I

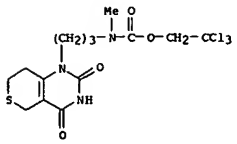
L4 ANSWER 10 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

AB Title compds. [I; A = O, CH2D, DCH2, CH:CHCH2, CH2CH:CH, CH2CH2D, DCH2CH2, CH2DCH2; D = CH2, O, S; X = (substituted) alkylene, cycloalkylene; R1 = H, (halogenated) alkyl, cycloalkyl; R2 = SO2R4, SO2NR5R6, COR7, CONR8R9, CO2R10; R4 = (substituted) alkyl, cycloalkyl, GE; E = (substituted) aryl, heterocyclyl, G is absent or (substituted) aryl, heteroaryl; R5, R6 = H, (substituted) cycloalkyl, alkyl, aryl, heteroaryl; or R5R6 = (substituted) heterocyclyl; R7 = (substituted) alkyl, cycloalkyl; GE (as above); R8, R9 = H, (substituted) alkyl, cycloalkyl; or R8R9 = (substituted) heteroaryl; R10 = (substituted) alkyl, cycloalkyl, aryl; or R1R2 = (substituted) mono- or bicyclic heterocyclyl; R3 = H, alkoxycarbonyl], were prepared Thus, a mixture of N-(3-aminopropyl)-N-benzyl-N-methylamine and tetrahydro-4H-thiopyran-4-one in PhMe was refluxed with camphorsulfonic acid followed by addition of ClCONCO at room temperature to give 67% 1-[3-benzyl(methyl)aminopropyl]-1,5,7,8-tetrahydro-2H-thiopyrano[4,3-d]pyrimidine-2,4(3H)-dione which was stirred with 2,2,2-trichloroethylchloroformate in MeCN for 30 min at room temperature to give 63% 2,2,2-trichloroethyl-3-(2,4-dioxo-3,4,7,8-tetrahydro-2H-thiopyrano[4,3-d]pyrimidin-1(5H)-yl)propyl(methyl)carbamate. Tested I showed 50% protection of endothelial cells with EC50 = 0.05-0.5 μM.

IT 390765-56-7P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of fused amidoalkyluracils as poly(ADP-ribose) synthetase inhibitors)

RN 390765-56-7 HCAPLUS

CN Carbamic acid, methyl[3-(3,4,7,8-tetrahydro-2,4-dioxo-2H-thiopyrano[4,3-d]pyrimidin-1(5H)-yl)propyl]-, 2,2,2-trichloroethyl ester (9CI) (CA INDEX NAME)



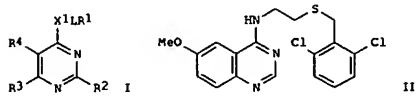
REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 11 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2001:338503 HCAPLUS
DOCUMENT NUMBER: 134:340517
TITLE: Preparation of heterocycles containing a 4-substituted pyrimidine subunit for pharmaceutical use as mGluR1 antagonists
INVENTOR(S): Ambler, Samantha Jayne; Baker, Stephen Richard; Clark, Barry Peter; Coleman, Darrell Stephen; Foglesong, Robert James; Goldsworthy, John; Jagdmann, Gunnar Erik, Jr.; Johnson, Kirk Willis; Kingston, Ann Elizabeth; Owton, William Martin; Schoepp, Darryle Darwin; Hong, Jian Eric; Schkeryantz, Jeffrey Michael; Vannieuwenhze, Michael Scott; Zia-Ebrahimi, Mohammad Sadegh
PATENT ASSIGNEE(S): Eli Lilly and Company, USA
SOURCE: PCT Int. Appl., 237 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001032632	A2	20010510	WO 2000-US26261	20001019
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
EP 1230225	A2	20020814	EP 2000-971987	20001019
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				
PRIORITY APPLN. INFO.:			US 1999-162900P	P 19991101
			WO 2000-US26261	W 20001019

OTHER SOURCE(S): MARPAT 134:340517
GI



I II

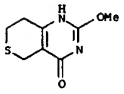
AB Heterocycles containing a 4-substituted pyrimidine subunit, such as I [R1 = carbocyclyl, heterocylyl; R2 = H, CN, SCH2CN, halogen, alkylthio, alkoxy, alkylsulfonyl, alkylamino, alkylsulfinyl, etc.; R3, R4 = alkyl; R3R4 = fused heterocycle, such as S(CH2)3, CH2O(CH2)2, CH:CHS, or fused carbocycle, such as CH:CHCH:CH, (CH2)4; L = alkylene or heteroalkylene linking group; X1 = O, NH], were prepd for pharmaceutical use as mGluR1

L4 ANSWER 11 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
antagonists for treatment of migraine. Thus, quinazolinine II was prepd. in three steps, which included cyclization of 2-amino-5-methoxybenzoic acid with formamidine to form 6-methoxy-4(1H)-quinazolinone, chlorination with phosphorus oxychloride to form 4-chloro-6-methoxyquinazoline followed by amination with 2-(2,6-dichlorobenzylthio)ethylamine. The prepd. pyrimidines were tested for mGluR1 and mGluR5 metabotropic glutamate receptor antagonist activity and were found to be 10 fold selective for the mGluR1 receptor.

IT **284028-92-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of heterocycles containing a 4-substituted pyrimidine subunit for
pharmaceutical use as mGluR1 antagonists for treatment of migraine)

RN 284028-92-8 HCAPLUS

CN 4H-Thiopyrano[4,3-d]pyrimidin-4-one, 1,5,7,8-tetrahydro-2-methoxy- (9CI) (CA INDEX NAME)



L4 ANSWER 12 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN

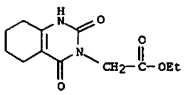
ACCESSION NUMBER: 2001:252578 HCAPLUS
DOCUMENT NUMBER: 135:61292
TITLE: Synthesis of new fused pyrimidines by isocyanate and isothiocyanate
AUTHOR(S): Chowdhury, A. Z. M. Shaifullah; Shibata, Yasuyuki
CORPORATE SOURCE: Environmental Chemistry Division, National Institute for Environmental Studies, Tsukuba, 305-0053, Japan
SOURCE: Chemical & Pharmaceutical Bulletin (2001), 49(4), 391-395
CODEN: CPBTAL; ISSN: 0009-2363
PUBLISHER: Pharmaceutical Society of Japan
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 135:61292

AB O-Amino nitrile or o-amino ester compds. were cyclized to fused pyrimidines by reacting with Et (isothiocyanato)acetate in pyridine, and then were methylated, halogenated and subsequently displaced by the amines studied. Reactants used in this study included 2-amino-4,5-dimethyl-3-furancarbonitrile, 2-amino-4,7-dihydro-5H-thieno[2,3-c]pyran-3-carbonitrile, 1-methyl-3-mercapto-1H-pyrazole-4-carbonitrile, 3-amino-1-methyl-1H-pyrazole-4-carbonitrile, 3-hydroxy-1-methyl-1H-pyrazole-4-carbonitrile, 2-amino-1-cyclopentene-1-carboxylic acid Et ester, 2-amino-1-cyclohexene-1-carboxylic acid Et ester, and 2-amino-4,7-dihydro-5H-thieno[2,3-c]pyran-3-carboxylic acid, Et ester.

IT **345897-26-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of fused pyrimidines by cyclocondensation of isocyanate and isothiocyanate derivs.)

RN 345897-26-9 HCAPLUS

CN 3(2H)-Quinazolineacetic acid, 1,4,5,6,7,8-hexahydro-2,4-dioxo-, ethyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 13 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN

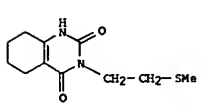
ACCESSION NUMBER: 2000:858982 HCAPLUS
DOCUMENT NUMBER: 134:162623
TITLE: Reactivity and Selectivity of Reactions of Small Radicals with a Multifunctional Heterocyclic Molecule: 3-(Mercaptoethyl)chinazoline-2,4-(1H,3H)dione
AUTHOR(S): Brede, O.; Schwinn, J.; Leistner, S.; Naumov, S.; Sprinz, H.
CORPORATE SOURCE: Interdisciplinary Group Time-Resolved Spectroscopy and Institute for Pharmacy, University of Leipzig, Leipzig, D-4303, Germany
SOURCE: Journal of Physical Chemistry A (2001), 105(1), 119-127
CODEN: JPCAFH; ISSN: 1089-5639
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Using pulse radiolysis, we studied the reactions of small radicals (e-aq, OH•, N3•, and •CH2OH) with the title compound in aqueous solution Whereas the solvated electron adds selectively to the carbonyl group near the aromatic moiety, the hydroxyl radical reacts by addition to the aromatic ring
as well as by H abstraction at >N(1)H and -SH groups. Also, azide radicals nonspecifically oxidize the aromatic ring, the thiol group, or the thiolate anion and the amine group at N(1), as identified by subsequent radical products. In contrast, hydroxymethyl radicals (derived from methanol) abstract hydrogen selectively at the thiol group. The thiyl radical formed was used to study the kinetics of H abstraction in the bis-allylic positions of linolenic acid. Product transient identification was performed by kinetic anal. as well as by comparison with reactions of mols. with structures less complex than that of the title compound, exhibiting relevant functional groups.

IT **324582-85-6**
RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(reactivity and selectivity of reactions of small radicals with 3-(mercaptoethyl)-2,4-(1H,3H)quinazolinedione)

RN 324582-85-6 HCAPLUS

CN 2,4(1H,3H)-Quinazolinedione, 5,6,7,8-tetrahydro-3-[2-(methylthio)ethyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 14 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN

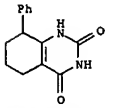
ACCESSION NUMBER: 2000:631373 HCAPLUS
DOCUMENT NUMBER: 134:29370
TITLE: Synthesis of annelated analogs of 6-benzyl-1-(ethoxymethyl)-5-isopropyluracil (MKC-442) using 1,3-oxazine-2,4(3H)-diones as key intermediates
AUTHOR(S): Larsen, Janus S.; Christensen, Lene; Ludvig, Gitte; Jorgensen, Per T.; Pedersen, Erik B.; Nielsen, Claus
CORPORATE SOURCE: Department of Chemistry, University of Southern Denmark, Odense, DK-5230, Den.
SOURCE: Perkin 1 (2000), (18), 3035-3038
CODEN: PERKF9
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 134:29370

AB Condensation of Et 3-phenyl-2-oxocyclopentanecarboxylate with 2-(S-methylthio)isourea followed by hydrolysis with HCl gave 6,7-dihydro-7-phenylcyclopenta[e][1,3]oxazine-2,4(3H,5H)-dione. 7,8-Dihydro-8-phenyl-6H-cyclohexa[e][1,3]oxazine-2,4(3H,5H)-dione was synthesized by reacting 2-phenylcyclohexanone with N-(chlorocarbonyl) isocyanate. These oxazines were treated with ammonia to obtain the corresponding uracil derivs., which after silylation were alkylated with diethoxymethane using trimethylsilyl triflate as the catalyst or alkylated with chloromethyl Et ether to give annelated MKC-442 analogs which are locked in a conformation close to the one of MKC-442. In spite of this, only moderate activities were found against HIV-1 for the annelated analogs of MKC-442.

IT **312312-86-0P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(preparation and virucidal activity of annelated 6-benzyl-1-(ethoxymethyl)-5-isopropyluracil (MKC-442) analogs)

RN 312312-86-0 HCAPLUS

CN 2,4(1H,3H)-Quinazolinedione, 5,6,7,8-tetrahydro-8-phenyl- (9CI) (CA INDEX NAME)

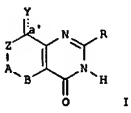


REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 15 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2000:493529 HCAPLUS
DOCUMENT NUMBER: 133:105047
TITLE: Preparation of pyrimidine derivatives as poly(ADP-ribose) polymerase inhibitors
INVENTOR(S): Hasegawa, Toshifumi; Nakajima, Hidemitsu; Kubota, Dai; Okuma, Kunihiro
PATENT ASSIGNEE(S): Meiji Seika Kaisha, Ltd., Japan
SOURCE: PCT Int. Appl., 67 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000042025	A1	20000720	WO 2000-JP153	20000114
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
EP 1142881	A1	20011010	EP 2000-900393	20000114
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				

PRIORITY APPLN. INFO.: JP 1999-8446 A 19990114
WO 2000-JP153 W 20000114
OTHER SOURCE(S): MARPAT 133:105047
GI



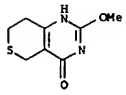
I

AB The title compds. I [R is hydrogen, C1-C8 alkyl, substituted C1-C8 alkyl, aryl, substituted aryl, aryl-substituted C1-C8 alkyl, or the like; Y is hydrogen or C(R2)R3 (wherein R2 and R3 are each hydrogen, C1-C8 alkyl, hydroxyalkyl(C1-C8), or the like), with the proviso that when Y is hydrogen, a' represents a single bond, and when Y is C(R2)R3, a' represents a double bond; A-B is CH2CH2, SCH2, etc.; and Z is CH2 or a single bond] are prepared 2-Methyl-3,5,7,8-tetrahydrothiopyrano[4,3-d]pyrimidin-4-one in vitro showed IC50 of 0.21 μM against poly(ADP-ribose) polymerase. Formulations are given.

IT 284028-92-8P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological

L4 ANSWER 15 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of pyrimidine derivs. as poly(ADP-ribose) polymerase inhibitors)

RN 284028-92-8 HCAPLUS
CN 4H-Thiopyrano[4,3-d]pyrimidin-4-one, 1,5,7,8-tetrahydro-2-methoxy- (9CI) (CA INDEX NAME)

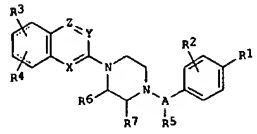


REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 16 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2000:186734 HCAPLUS
DOCUMENT NUMBER: 132:222551
TITLE: Preparation of 1-(2-naphthyl)- and 1-(2-azanaphthyl)-4-(1-phenylmethyl)piperazines as dopamine receptor subtype specific ligands
INVENTOR(S): Greenlee, William; Gangly, Ashit; Wasley, Jan W. F.
PATENT ASSIGNEE(S): Neurogen Corporation, USA
SOURCE: U.S., 12 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6040448	A	20000321	US 1998-177956	19981023
US 6331629	B1	20011218	US 2000-522139	20000309
US 2002013317	A1	20020131	US 2001-897352	20010702
US 6384224	B2	20020507		

PRIORITY APPLN. INFO.: US 1997-63149P P 19971024
US 1998-177956 A3 19981023
US 2000-522139 A1 20000309
OTHER SOURCE(S): MARPAT 132:222551
GI



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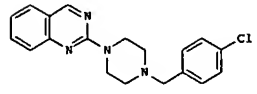


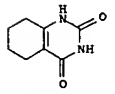
II

AB The title compds. [I; X, Y, Z = (un)substituted C, N; R1, R2 = H, F, Cl, etc.; R3, R4 = H, halo, alkyl, etc.; R5-R7 = H, alkyl; A = alkylene] and their pharmaceutically acceptable addition salts which bind selectively with high affinity to the dopamine D4 receptor subtype and are therefore are useful in treatment of various neuropsychol. disorders were prepared E.g., a 4-step synthesis of II.HCl, starting with benzoyleneurea, was presented. Biol. data (Ki against D4 and D2 receptor binding) for compds. I were given.

IT 35042-48-9, 5,6,7,8-Tetrahydro-2,4(1H,3H)-quinazolinedione

L4 ANSWER 16 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of 1-(2-naphthyl)- and 1-(2-azanaphthyl)-4-(1-phenylmethyl)piperazines as dopamine receptor subtype specific ligands)

RN 35042-48-9 HCAPLUS
CN 2,4(1H,3H)-Quinazolinedione, 5,6,7,8-tetrahydro- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 17 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN

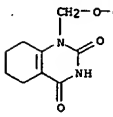
ACCESSION NUMBER: 1999:799126 HCAPLUS
DOCUMENT NUMBER: 132:102526
TITLE: Further studies on cytostatic activity of alkoxymethyl purine and pyrimidine acyclonucleosides
AUTHOR(S): Modrzejewska, Hanna; Draminski, Marcin; Zgit-Wroblewska, Anna; Greger, Janusz
CORPORATE SOURCE: Department of Biochemistry, Institute of Physiology and Biochemistry, Medical University of Lodz, Lodz, 90-131, Pol.
SOURCE: Zeitschrift fuer Naturforschung, C: Journal of Biosciences (1999), 54(11), 923-931
CODEN: ZNCBDA; ISSN: 0939-5075
PUBLISHER: Verlag der Zeitschrift fuer Naturforschung
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The influence of 14 acyclonucleosides, derivs. of adenine, guanine, uracil and thymine on the phosphorylation of dAdo, dGuo, dCyd and dThd occurring in the cytosol of growing amelanotic melanoma transplanted to Syrian hamsters, as well as on inhibition of tumor growth were studied. From among the studied ACNs eight were tested earlier. The influence of alkoxymethyl purine and pyrimidine acyclonucleosides on growth inhibition of Kirkman-Robbins hepatoma and possible mechanism of their cytostatic activity, from among the newly synthesized ACNs, 1,3-N,N-diallyoxymethylthymine (AMT2), 1-N-allyloxymethyl-5,6-tetramethyleneuracil (AMUTM), and tested previously 1-N-allyloxymethylthymine (AMT1), administered i.p. in a dose of 0.2 mmol /kg body weight reduce the tumor mass from 0.98 g to 0.64 g ± 0.11 g (i.e. 35% ± 12%). 48 H after i.p. administration of the mentioned ACNs in the same dose a reduction of tumor mass is accompanied by the inhibition of dAMP, dGMP and dTMP synthesis. AMT1 inhibits dThd phosphorylation from 6.2 to 4.22; AMT2 suppresses dAdo, dGuo and dThd phosphorylation by, correspondingly, from 2.8 to 1.7, from 10.8 to 7.5 and from 6.2 to 4.2; AMUTM depresses dAMP synthesis from 2.8 to 1.6 (all data: μmol of 2'dNMP formed per mg of protein per min. + 10-4). None of the 14 studied acyclonucleosides influences dCMP synthesis. In vivo, after hydration of allyloxymethyl group to hydroxypropoxymethyl residue (having -CH2OH group), AMT1, AMT2 and AMUTM undergo phosphorylation to corresponding triphosphates. Phosphorylated ACNs are not incorporated into tumor DNA, however they inhibit dAdo, dGuo and dThd incorporation into DNA. It is concluded that ACN triphosphates are not substrates for DNA polymerase but, competing with dATP dGTP and dTTP, inhibit incorporation of these 2'dNTP into DNA and, in consequence, reduce tumor growth, which is presumed to be the main mechanism of cytostatic activity of the studied ACNs.

IT **255911-46-7P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and effect of acylnucleoside triphosphates on phosphorylation of dATP dGTP and dTTP, and melanoma growth)

RN 255911-46-7 HCAPLUS
CN 2,4(1H,3H)-Quinazolinedione, 5,6,7,8-tetrahydro-1-[(2-propenyloxy)methyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 17 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

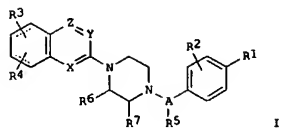
L4 ANSWER 18 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1999:297415 HCAPLUS
DOCUMENT NUMBER: 130:311822
TITLE: Preparation of 1-(2-naphthyl)- and 1-(2-azanaphthyl)-4-(1-phenylmethyl)piperazines as dopamine D4 receptor subtype ligands
INVENTOR(S): Greenlee, William; Ganguly, Ashit; Wasley, Jan W. F.
PATENT ASSIGNEE(S): Neurogen Corporation, USA; Schering Corporation
SOURCE: PCT Int. Appl., 56 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

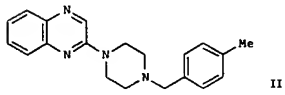
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9921850	A1	19990506	WO 1998-US22233	19981021
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2308057	AA	19990506	CA 1998-2308057	19981021
AU 9898104	A1	19990517	AU 1998-98104	19981021
EP 1025097	A1	20000809	EP 1998-952391	19981021
EP 1025097	B1	20050427		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
AT 294173	E	20050515	AT 1998-952391	19981021
ES 2241172	T3	20051016	ES 1998-952391	19981021
ZA 9809720	A	19990426	ZA 1998-9720	19981026
PRIORITY APPLN. INFO.:			US 1997-954353	A2 19971024
			WO 1998-US22233	W 19981021

OTHER SOURCE(S): MARPAT 130:311822
GI

L4 ANSWER 18 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



I

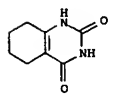


II

AB The title compds. [I: X, Y, Z = CH, C(halo), C(alkyl), N; R1, R2 = H, halo, OH, etc.; R1R2 = C1-2 alkylene dioxy, C1-3 alkylene oxy; R3, R4 = H, halo, alkyl, etc.; A = C1-4 alkylene; R5-R7 = H, alkyl] and their salts which bind selectively with high affinity to the dopamine D4 receptor subtype and are therefore of use in treatment of various neuropsychol. disorders, were prepared Thus, treatment of 2-hydroxyquinoxaline with POCl3 followed by reaction of the crude chloride with piperazine, and alkylation of quinoxalin-2-ylpiperazine with 4-methylbenzyl bromide afforded II which showed Ki of 8 nM against binding to D4 receptor cloned from African Green monkey.

IT **35042-48-9**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of 1-(2-naphthyl)- and 1-(2-azanaphthyl)-4-(1-phenylmethyl)piperazines as dopamine D4 receptor subtype ligands)

RN 35042-48-9 HCAPLUS
CN 2,4(1H,3H)-Quinazolinedione, 5,6,7,8-tetrahydro- (9CI) (CA INDEX NAME)

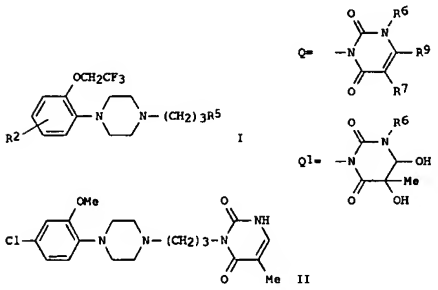


REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 19 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1999:45146 HCAPLUS
DOCUMENT NUMBER: 130:125098
TITLE: Preparation of pyrimidinedione, pyrimidinetrione, triazinedione and tetrahydroquinazolinedione derivatives as α1-adrenergic receptor antagonists
INVENTOR(S): Bantle, Gary W.; Elworthy, Todd R.; Guzman, Angel; Jaime-Figueroa, Saul; Lopez-Tapia, Francisco J.; Morgans, David J., Jr.; Perez-Medrano, Arturo; Pfister, Jurg R.; Sjogren, Eric B.; Talamas, Francisco X.
PATENT ASSIGNEE(S): Syntex (U.S.A.) Inc., USA
SOURCE: U.S., 36 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

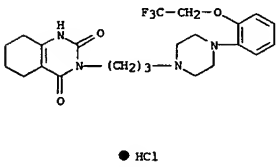
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5859014	A	19990112	US 1996-658774	19960605

PRIORITY APPLN. INFO.: US 1996-658774 19960605
OTHER SOURCE(S): MARPAT 130:125098
GI



AB The title compds. of formula, in particular, [I; R2 = H, Cl, F, OH, Me; R5 = Q, Q1; wherein R6 = H, Me, cyclohexylmethyl, pyridylmethyl, pyrazinylmethyl, furylmethyl, thienylmethyl, biphenylmethyl, (un)substituted Ph or benzyl] or pharmaceutically acceptable salts and

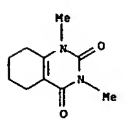
L4 ANSWER 19 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
N-oxides thereof, are prepd. These compds. are α1-adrenergic receptor antagonists and are useful for the treatment of diseases involving directly or indirectly an obstruction of the lower urinary tract, such as benign prostatic hyperplasia. Thus, a mixt. of 3-(3-chloropropyl)-5-methyl-2,4(1H,4H)-pyrimidinedione (prepn. given) and 1-(4-chloro-2-methoxyphenyl)piperazine (prepn. given) were heated with stirring at 180-190° for 2 h to give the title compd. (II). Compds. of formula I were tested in vitro and found to selectively inhibit the α1-adrenoceptor mediated contractions of human, isolated prostatic and bladder neck smooth muscle (no detailed data given). In contrast, prazosin non-selectively inhibited the α1-adrenoceptor-mediated contractions of both human, isolated prostatic/bladder neck smooth muscle and isolated arterial smooth muscle.
IT 186386-03-8P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyrimidinedione, pyrimidinetrione, triazinedione and tetrahydroquinazolinedione derivs. as α1-adrenergic receptor antagonists for treatment of urinary tract diseases)
RN 186386-03-8 HCAPLUS
CN 2,4(1H,3H)-Quinazolinedione, 5,6,7,8-tetrahydro-3-[3-[4-[2-(2,2,2-trifluoroethoxy)phenyl]-1-piperazinyl]propyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 20 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1998:517094 HCAPLUS
DOCUMENT NUMBER: 129:241357
TITLE: Partial molar volumes of alkylated uracils- insight into the solvation shell? Part II
AUTHOR(S): Zielenkiewicz, W.; Poznanski, J.; Zielenkiewicz, A.
CORPORATE SOURCE: Inst. Physical Chemistry, Polish Academy Sciences, Warsaw, 01-224, Pol.
SOURCE: Journal of Solution Chemistry (1998), 27(6), 543-551
CODEN: JSLCAG; ISSN: 0095-9782
PUBLISHER: Plenum Publishing Corp.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The solute-solvent interactions in aqueous solns. of alkylated uracils are discussed. The partial molar volume data are interpreted using a new model of interaction of the solute mol. with the solvent. The model is based on the assumption that the d. of solvent in the hydration shell depends on the structure and polarity of the solute mol. The relation among mol. volume, partial molar volume, and volume of the solvation shell is expressed by a parameter, which is defined as the relative d. of the solvation shell. It is found that in compds. with the same number of CH2-groups, the α values depend on substitution on the C or N atoms of the uracil skeleton. The α values also depend to some extent, on screening of the oxygen atoms by methylation of the neighboring atoms of the uracil ring. A correlation is presented between the relative d. of solvation shell and polarity (defined as the ratio of the surface of polar groups and atoms exposed to the solvent to the total accessible mol. surface of the mol.) for the compds. studied. It was demonstrated that of the various solute-solvent interactions the dominant role is played by polar interactions.
IT 80254-48-4
RL: PRP (Properties)
(partial molar volumes of alkylated uracils and insight into the solvation shell)
RN 80254-48-4 HCAPLUS
CN 2,4(1H,3H)-Quinazolinedione, 5,6,7,8-tetrahydro-1,3-dimethyl- (9CI) (CA INDEX NAME)



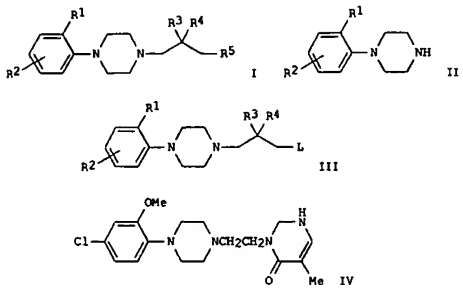
REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 21 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1997:124395 HCAPLUS
DOCUMENT NUMBER: 126:131468
TITLE: Preparation of pyrimidinedione, pyrimidinetrione, triazinedione, and tetrahydroquinazolinedione derivatives as α1-adrenoceptor antagonists
INVENTOR(S): Bantle, Gary W.; Elworthy, Todd R.; Guzman, Angel; Jaime-figueroa, Saul; Lopez-Tapia, Francisco J.; Morgans, David J., Jr.; Perez-Medrano, Arturo; Pfister, Juerg R.; Sjogren, Eric B.; Talamas, Francisco X.
PATENT ASSIGNEE(S): F. Hoffmann-La Roche Ag, Switz.
SOURCE: Eur. Pat. Appl., 51 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 748800	A2	19961218	EP 1996-108493	19960528
EP 748800	A3	19961227		
EP 748800	B1	20010509		
R: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
AT 201016	E	20010515	AT 1996-108493	19960528
ES 2157366	T3	20010816	ES 1996-108493	19960528
PT 748800	T	20011030	PT 1996-108493	19960528
IL 118519	A1	19991222	IL 1996-118519	19960531
ZA 9604561	A	19961209	ZA 1996-4561	19960603
AU 9654690	A1	19961219	AU 1996-54690	19960603
AU 710754	B2	19990930		
PL 188061	B1	20041231	PL 1996-314635	19960605
CA 2178548	AA	19961210	CA 1996-2178548	19960607
NO 9602412	A	19961210	NO 1996-2412	19960607
NO 309424	B1	20010129		
JP 09100269	A2	19970415	JP 1996-145236	19960607
JP 2721147	B2	19980304		
CN 1149051	A	19970507	CN 1996-110490	19960607
CN 1118459	B	20030820		
BR 9602705	A	19980908	BR 1996-2705	19960607
RU 2175322	C2	20011027	RU 1996-111418	19960607
CZ 290004	B6	20020515	CZ 1996-1696	19960610
HK 1013065	A1	20020125	HK 1998-114167	19981221
GR 3036307	T3	20011031	GR 2001-401157	20010731

PRIORITY APPLN. INFO.: US 1995-489183 A 19950609
OTHER SOURCE(S): MARPAT 126:131468
GI

L4 ANSWER 21 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



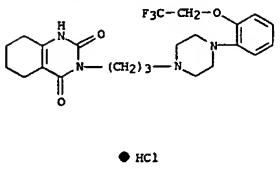
AB The title compds. (I; R1 = AcNH, NH, cyano, CF3CONH, halo, H, OH, NO2, 2-propynyloxy, etc.; R2 = cyano, halo, H, OH, etc.; R3, R4 = H, Me, CH2CH2; R5 = N-containing heterocyclyl) and the pharmaceutically acceptable salts and N-oxides thereof are prepared by reacting pyrazine derivs. (II; R1, R2 = same as above) with LCH2CR3R4R5 (R3, R4, R5 = same as above; L = leaving group) or reacting pyrazine derivs. (III; R1, R2, R3, R4, L = same as above) with H-R5 (R5 = same as above). I, possessing α1-adrenoceptor antagonism, are useful for treatment of a disease involving (in)directly an obstruction of the lower urinary tract caused by benign prostatic hyperplasia. Thus, a mixture of 3-(3-chloropropyl)-5-methyl-2,4(1H,3H)pyrimidinedione (preparation given) and 1-(4-chloro-2-methoxyphenyl)piperazine (preparation given) was heated at 180-190° to give the title compound (IV). I selectively inhibited α1-adrenoceptor when tested on rabbit, rat, and human in vitro.

IT **186386-03-8P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyrimidinedione, pyrimidinetrione, triazinedione, and tetrahydroquinazolinedione derivs. as α1-adrenoceptor antagonists)

RN 186386-03-8 HCAPLUS

CN 2,4(1H,3H)-Quinazolinedione, 5,6,7,8-tetrahydro-3-[3-[4-[2-(2,2,2-trifluoroethoxy)phenyl]-1-piperazinyl]propyl]-, monohydrochloride (9CI) (CA INDEX NAME)

L4 ANSWER 21 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



● HCl

L4 ANSWER 22 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN

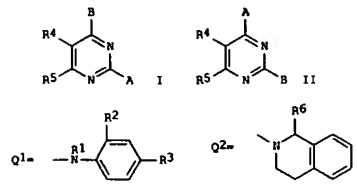
ACCESSION NUMBER: 1996:401560 HCAPLUS
DOCUMENT NUMBER: 125:58535
TITLE: Preparation of pyrimidine derivatives as gastric secretion inhibitors
INVENTOR(S): Lee, Jong Wook; Chae, Jeong Seok; Kim, Chang Seop; Kim, Jae Kyu; Lim, Dae Sung; Shon, Moon Kyu; Choi, Yeon Shik; Lee, Sang Ho
PATENT ASSIGNEE(S): Yuhan Corporation, S. Korea
SOURCE: PCT Int. Appl., 93 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9605177	A1	19960222	WO 1995-KR105	19950810
W: AU, CA, CN, JP, RU, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
KR 157075	B1	19981116	KR 1994-19997	19940813
KR 157076	B1	19981116	KR 1994-19998	19940813
CA 2197298	AA	19960222	CA 1995-2197298	19950810
CA 2197298	C	19991019		
AU 9531225	A1	19960307	AU 1995-31225	19950810
AU 688087	B2	19980305		
EP 775120	A1	19970528	EP 1995-927092	19950810
EP 775120	B1	20030604		
R: CH, DE, ES, FR, GB, IT, LI, SE				
CN 1155281	A	19970723	CN 1995-194599	19950810
CN 1102144	B	20030226		
JP 09509188	T2	19970916	JP 1995-507208	19950810
JP 2896532	B2	19990531		
RU 2129549	C1	19990427	RU 1997-104208	19950810
ES 2201112	T3	20040316	ES 1995-927092	19950810
US 5750531	A	19980512	US 1997-776220	19970123
HK 1001618	A1	20030822	HK 1998-100535	19980121

PRIORITY APPLN. INFO.:

KR 1994-19997	A	19940813
KR 1994-19998	A	19940813
WO 1995-KR105	W	19950810

OTHER SOURCE(S): MARPAT 125:58535
GI



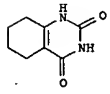
L4 ANSWER 22 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

AB The title compds. I and II [R4 and R5, which may be the same or different, are independently hydrogen or a C1-C3 alkyl group, or jointly form a cyclopentyl or cyclohexyl ring; A is Q1 wherein R1 and R2 are, independently of each other, hydrogen or a C1-C3 alkyl group, and R3 is hydrogen, a C1-C3 alkyl group or a halogen; and B is Q2, etc.; R6 is hydrogen or a C1-C3 alkyl group] are prepared 2-(2-Methyl-4-fluorophenylamino)-4-(1-methyl-1,2,3,4-tetrahydroisoquinolin-2-yl)pyrimidine hydrochloride (preparation given) in vitro showed IC50 of 5.4 μM against H+/K+ ATPase, vs. 5.8 μM for omeprazole. The inhibition of enzyme activity by compds. of this invention is reversible.

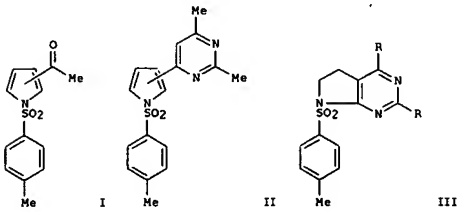
IT **35042-48-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of pyrimidine derivs. as gastric secretion inhibitors)

RN 35042-48-9 HCAPLUS

CN 2,4(1H,3H)-Quinazolinedione, 5,6,7,8-tetrahydro- (9CI) (CA INDEX NAME)

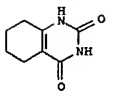


L4 ANSWER 23 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1996:355014 HCAPLUS
DOCUMENT NUMBER: 125:142661
TITLE: New procedures for the synthesis of heterocyclic substituted and 2,4-difunctionalized pyrimidines
AUTHOR(S): Garcia Martinez, Antonio; Herrera Fernandez, Antonio; Moreno Jimenez, Florencio; Munoz Martinez, Pablo J.; Alonso Martin, Cristina; Subramanian, Laksminarayanapuran R.
CORPORATE SOURCE: Dep. Quim. Org., Fac. Cienc. Quim., Univ. Complutense, Madrid, E-28040, Spain
SOURCE: Tetrahedron (1996), 52(23), 7973-7982
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 125:142661
GI

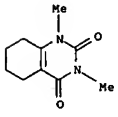


AB N-Tosyl-2- and 3-acetylpyrroles I or N-tosyl-2-pyrrolidone were condensed with cyano compds. in the presence of triflic anhydride (Tf2O) to yield heteroacylpyrimidines II and III (R = Me, SMe), resp. 2,4-Difunctionalized pyrimidines, e.g., IV [R1 = Me, R2 = Me, Et; R1R2 = (CH2)4, (CH2)5], were obtained by reaction of the corresponding 2,4-bis(methylsulfonyl)pyrimidines with nucleophiles.
IT 35042-48-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of pyrimidines)
RN 35042-48-9 HCAPLUS
CN 2,4(1H,3H)-Quinazolinedione, 5,6,7,8-tetrahydro- (9CI) (CA INDEX NAME)

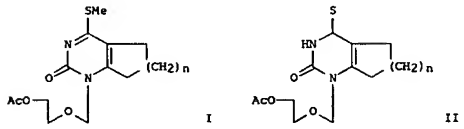
L4 ANSWER 23 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



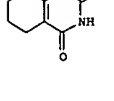
L4 ANSWER 24 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1995:908410 HCAPLUS
DOCUMENT NUMBER: 124:116944
TITLE: Thermochemistry of aqueous solutions of nucleic acid bases and their alkylated derivatives
AUTHOR(S): Zielenkiewicz, W.
CORPORATE SOURCE: Inst. Physical Chem., Polish Academy of Sciences, Warsaw, 01-224, Pol.
SOURCE: Journal of Thermal Analysis (1995), 45(4), 615-29
CODEN: JTHEA9; ISSN: 0368-4466
PUBLISHER: Akademiai Kiado
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Enthalpy of solution, ΔH'sol, enthalpy of sublimation, ΔH'subl, apparent partial molar volume and heat capacities, V'2 and C'p,2 were determined for aqueous solns. of thirty alkylated derivs. of uracil and adenine, eight derivs. of cytosine and guanine. Calculated accessible surface areas and molar volumes are presented, too. The values of enthalpy of solution, enthalpy of sublimation can be useful in the studies on the nature of interaction between these compds. and water mols. Apparent partial molar volume and heat capacity give a new aspect on hydrophobic properties of the examined nucleic acid base derivs.
IT 80254-48-4
RL: PRP (Properties)
(thermochem. of aqueous solns. of nucleic acid bases and their alkylated derivs.)
RN 80254-48-4 HCAPLUS
CN 2,4(1H,3H)-Quinazolinedione, 5,6,7,8-tetrahydro-1,3-dimethyl- (9CI) (CA INDEX NAME)



L4 ANSWER 25 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1995:14213 HCAPLUS
DOCUMENT NUMBER: 122:81839
TITLE: Synthesis and antiviral study of cyclopentano[d]pyrimidine-2,4-diones and octahydroquinazoline-2,4-diones acyclic nucleosides as potential anti-HIV agents
AUTHOR(S): Renault, Jacques; Laduree, Daniel; Robba, Max
CORPORATE SOURCE: Cent. Etud. Rech. Med. Norm., U.F.R. Sci. Pharm., Caen, 14000, Fr.
SOURCE: Nucleosides & Nucleotides (1994), 13(4), 891-901
CODEN: NUNUD5; ISSN: 0732-8311
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



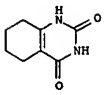
AB The Vorbruggen and Niedballa's method afforded new cyclopentano [d] pyrimidine-2,4-dione and octahydroquinazoline-2,4-dione nucleosides. Various modifications of these new derivs. enabled the authors to obtain HEPT related compds., e.g. I and II (n = 1, 2), which were tested against Human Immunodeficiency Virus-1 (HIV-1). Unfortunately, none of these compds. showed significant antiviral activity.
IT 35042-48-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, in synthesis of cyclopentanopyrimidine-2,4-dione and octahydroquinazoline-2,4-dione nucleosides)
RN 35042-48-9 HCAPLUS
CN 2,4(1H,3H)-Quinazolinedione, 5,6,7,8-tetrahydro- (9CI) (CA INDEX NAME)



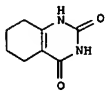
L4 ANSWER 26 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1994:655511 HCAPLUS
DOCUMENT NUMBER: 121:255511
TITLE: Preparation of (cycloalkapyrimidiniothiomethyl)cephalosporin antibacterials.
INVENTOR(S): Bang, Chan-Sik; Kim, Yong-Zu; Yeo, Jae-Hong; Lim, Jong-Chan; Oh, Hun-Seung; Woo, Young-Min; Yang, Duk-Ho; Kim, Sam-Sik; Yim, Hyeon-Joo
PATENT ASSIGNEE(S): Lucky Ltd., S. Korea
SOURCE: Eur. Pat. Appl., 26 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 604920	A1	19940706	EP 1993-120829	19931223
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
KR 154901	B1	19981116	KR 1992-25647	19921226
US 5416081	A	19950516	US 1993-171535	19931222
JP 06211872	A2	19940802	JP 1993-330684	19931227
JP 08011757	B4	19960207		
PRIORITY APPLN. INFO.:			KR 1992-25647 A	19921226
OTHER SOURCE(S):		MARPAT 121:255511		

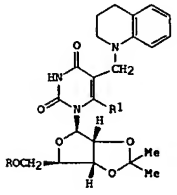
GI For diagram(s), see printed CA Issue.
AB Title compds. [I; R1 H, C1-4 alkyl, C2-4 alkenyl, C2-4 alkynyl, C(RA)(RB)COOH; RA, RB = H, C1-4 alkyl; CRARB = C3-7 cycloalkyl; R2 = (substituted) amino, C1-4 alkyl, C3-7 cycloalkyl; n = 2-7], were prepared Thus, paramethoxybenzyl 3-chloromethyl-7-[(Z)-2-(2-tert-butoxycarbonylprop-2-oxyimino)-2-[2-(triphenylmethyl)aminothiazol-4-yl]acetamido]-3-cephem-4-carboxylate and 1,4-diamino-1,5,6,7-tetrahydrocyclopentapyrimidine-2-thione (preparation given) were stirred in Me2SO to give a coupling product which was stirred with HCl in PhOH to give I (R = CMe2CO2H, R2 = NH2, n = 3). The latter showed a min. inhibitory concentration of 0.5 μg/mL against Pseudomonas aeruginosa.
IT **35042-48-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as intermediate for (cycloalkapyrimidiniothiomethyl)cephalosporin antibacterial)
RN 35042-48-9 HCAPLUS
CN 2,4(1H,3H)-Quinazolinedione, 5,6,7,8-tetrahydro- (9CI) (CA INDEX NAME)



L4 ANSWER 27 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1994:457445 HCAPLUS
DOCUMENT NUMBER: 121:57445
TITLE: Oxidation of substituted 2-thiouracils and pyrimidine-2-thione with ozone and 3,3-dimethyl-1,2-dioxirane
AUTHOR(S): Claudia, Crestini; Mincione, Enrico; Saladino, Raffaele; Nicoletti, Rosario
CORPORATE SOURCE: Dip. Chim., Univ. Roma "La Sapienza", Rome, 00185, Italy
SOURCE: Tetrahedron (1994), 50(10), 3259-72
CODEN: TETRAB; ISSN: 0040-4020
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Ozone and 3,3-dimethyl-1,2-dioxirane react with substituted 2-thiouracils and pyrimidine-2-thione to afford several desulfurized products. The effect of the solvent, protic as opposed to nonprotic, on the course of oxidation was striking.
IT **35042-48-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 35042-48-9 HCAPLUS
CN 2,4(1H,3H)-Quinazolinedione, 5,6,7,8-tetrahydro- (9CI) (CA INDEX NAME)



L4 ANSWER 28 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1993:512035 HCAPLUS
DOCUMENT NUMBER: 119:112035
TITLE: A chemical model for the fragmentation reaction in thymidylate synthase catalysis. Synthesis and evaluation of a 5-methylene-1-(1,2,3,4-tetrahydroquinolyl)-6-allyluridine
AUTHOR(S): Kagel, John R.; Wang, Binghe; Mertes, Mathias P.
CORPORATE SOURCE: Dep. Med. Chem., Univ. Kansas, Lawrence, KS, 66045, USA
SOURCE: Journal of Organic Chemistry (1993), 58(10), 2738-46
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

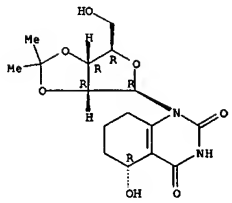


I, R=R1=H
II, R=SiMe2CMe3, R1=CH2CH=CH2

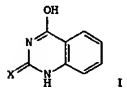
AB Nucleosides I and II were synthesized as models to investigate the reactivity of proposed intermediate in thymidylate synthase (TS) catalysis as it fragments to form dTMP. The mechanism of the fragmentation (homolytic or heterolytic) of model II was determined via subsequent interaction of the fragmented center with the C6 allyl substituent. The results were consistent with an ionic fragmentation of II, followed by loss of an allylic proton, and subsequent thermal electrocyclic or Diels-Alder reactions of the resulting trienes.
IT **126740-11-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and dehydration of)
RN 126740-11-2 HCAPLUS
CN 2,4(1H,3H)-Quinazolinedione, 5,6,7,8-tetrahydro-5-hydroxy-1-[2,3-O-(1-methylethylidene)-β-D-ribofuranosyl]-, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 28 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

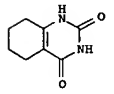


L4 ANSWER 29 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1993:428095 HCAPLUS
DOCUMENT NUMBER: 119:28095
TITLE: Ozonation of substituted 2-thiouracils and pyrimidine-2-thione
AUTHOR(S): Crestini, Claudia; Saladino, Raffaele; Nicoletti, Rosario
CORPORATE SOURCE: Dip. Chim., Univ. Roma La Sapienza, Rome, 00100, Italy
SOURCE: Tetrahedron Letters (1993), 34(10), 1631-4
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 119:28095
GI

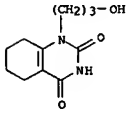


I

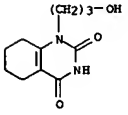
AB The ozonation of substituted 2-thiouracils and pyrimidine-2-thione, e.g., I (X = S) is reported; this provides a new method for the synthesis of several pyrimidine derivs. E.g., I (X = S) underwent ozonation in acetic acid-water to give quinazolindione I (X = O) in 75%. I (X = S) underwent ozonation in acetic acid alone to give quinazolinone I (X = H) in 82%.
IT 35042-48-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 35042-48-9 HCAPLUS
CN 2,4(1H,3H)-Quinazolinedione, 5,6,7,8-tetrahydro- (9CI) (CA INDEX NAME)



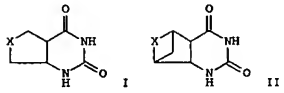
L4 ANSWER 30 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1992:590187 HCAPLUS
DOCUMENT NUMBER: 117:190187
TITLE: Phosphorylation of acyclonucleosides by nucleoside phosphotransferase from higher plants and bacteria
AUTHOR(S): Rutkowski, Maciej; Draminski, Marcin
CORPORATE SOURCE: Inst. Basic Sci., Mil. Med. Acad., Lodz, 90-647, Pol.
SOURCE: Acta Biochimica Polonica (1991), 38(4), 449-57
CODEN: ABPLAF; ISSN: 0001-527X
DOCUMENT TYPE: Journal
LANGUAGE: English
AB New pyrimidine acyclonucleosides were phosphorylated by nucleoside phosphotransferase from wheat shoots as well as from Enterobacter agglomerans. Conditions and parameters of enzymic phosphorylation were optimized and the results obtained with the 2 phosphotransferases were compared.
IT 72458-91-4
RL: BIOL (Biological study)
(phosphorylation of, by nucleoside phosphotransferase)
RN 72458-91-4 HCAPLUS
CN 2,4(1H,3H)-Quinazolinedione, 5,6,7,8-tetrahydro-1-(3-hydroxypropyl)- (9CI) (CA INDEX NAME)



L4 ANSWER 31 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1992:527964 HCAPLUS
DOCUMENT NUMBER: 117:127964
TITLE: Biotransformation, by Enterobacter agglomerans, of pyrimidine acyclonucleosides to acyclonucleotides
AUTHOR(S): Rutkowski, M.; Korczak, E.
CORPORATE SOURCE: Inst. Basic Sci., Mil. Med. Acad., Lodz, 90-647, Pol.
SOURCE: Experientia (1992), 48(6), 600-3
CODEN: EXPEAM; ISSN: 0014-4754
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The ability of Enterobacter agglomerans to transform naturally occurring nucleosides was utilized to transform newly synthesized pyrimidine acylonucleosides into the corresponding acylonucleotides. Unselected bacteria were used as the source of nucleoside phosphotransferase, the phosphate group donor being 4-nitrophenyl phosphate in the presence of Zn2+. Optimal reaction conditions are outlined.
IT 72458-91-4
RL: PROC (Process)
(transformation of, by Enterobacter agglomerans)
RN 72458-91-4 HCAPLUS
CN 2,4(1H,3H)-Quinazolinedione, 5,6,7,8-tetrahydro-1-(3-hydroxypropyl)- (9CI) (CA INDEX NAME)

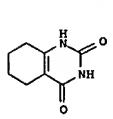


L4 ANSWER 32 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1992:511559 HCAPLUS
DOCUMENT NUMBER: 117:111559
TITLE: Stereochemical studies. 159. Preparation of uracil by cycloreversion. Structure of cycloalkane/ene- and norbornane/ene-fused dihydrouracils
AUTHOR(S): Frimpong-Manso, Samuel; Nagy, Katalin; Stajer, Geza; Bernath, Gabor; Sohar, Pal
CORPORATE SOURCE: Inst. Pharm. Chem., Albert Szent-Gyorgyi Med. Univ., Szeged, H-6701, Hung.
SOURCE: Journal of Heterocyclic Chemistry (1992), 29(1), 221-4
CODEN: JHTCAD; ISSN: 0022-152X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 117:111559
GI



I II

AB The reactions of the 2-amino-1-cycloalkane-, cycloalkene-, norbornane- and norbornenecarboxylates with potassium cyanate gave urea esters, which were cyclized to cycloalkane-, cycloalkene-, norbornane- and norbornene-fused 5,6-dihydrouracils I and II (X = CH2, CH2CH2, CH:CH). On cyclization, the urea ester formed from trans-4-cyclohexene-1-carboxylate, furnished the cis-fused 5,6-dihydropyrimidine-2,4(1H,3H)-dione I (X = CH:CH). On heating, the norbornene-di-exo-fused dihydrouracil II (X = CH:CH) yielded 2,4-pyrimidinedione through the splitting-off of cyclopentadiene. The structures of the prepared compds. were proved by 1H and 13C nmr spectroscopy.
IT 35042-48-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 35042-48-9 HCAPLUS
CN 2,4(1H,3H)-Quinazolinedione, 5,6,7,8-tetrahydro- (9CI) (CA INDEX NAME)

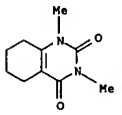


L4 ANSWER 33 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1992:160049 HCAPLUS
DOCUMENT NUMBER: 116:160049
TITLE: Apparent molar heat capacities and volumes of some alkylated derivatives of uracil and adenine in aqueous solution at 25°C
AUTHOR(S): Zielenkiewicz, Wojciech; Zielenkiewicz, Anna; Grolier, Jean Pierre E.; Roux, Alain H.; Roux-Desgranges, Genevieve
CORPORATE SOURCE: Inst. Phys. Chem., Pol. Acad. Sci., Warsaw, Pol.
SOURCE: Journal of Solution Chemistry (1992), 21(1), 1-13
CODEN: JSLCAG; ISSN: 0095-9782
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Densities and apparent molar heat capacities of some alkylated derivs. of uracil and adenine: 1-methyluracil, 1,3-dimethyluracil, 1,3-diethylthymine, 5,6-trimethylene-1,3-dimethyluracil, 5,6-tetramethylene-1,3-dimethyluracil, 5,6-pentamethylene-1,3-dimethyluracil, 2,9-dimethyladenine, 2-ethyl-9-methyladenine, 2-propyl-9-methyladenine, 8-ethyl-9-methyladenine, 6,8,9-trimethyladenine and 8-ethyl-6,9-dimethyladenine were determined using flow calorimetry and flow densimetry at 25°C. The partial molar volumes and heat capacities correlated linearly with the number of substituted methylene groups-CH2- as well as to the number of hydrogen atoms, nH, belonging to the skeleton of the mol. In the case of alkylated uracils, a difference was observed in the values at infinite dilution, V°2 and C°p2, depending on the substitution of alkyl and cyclooligomethylene groups.

IT **80254-48-4**
RL: PRP (Properties)
(apparent molar volumes and heat capacity of aqueous)

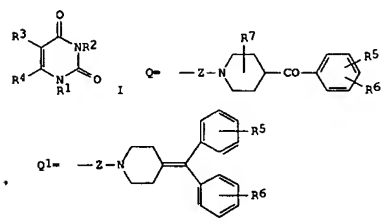
RN 80254-48-4 HCAPLUS
CN 2,4(1H,3H)-Quinazolinedione, 5,6,7,8-tetrahydro-1,3-dimethyl- (9CI) (CA INDEX NAME)



L4 ANSWER 34 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1992:151788 HCAPLUS
DOCUMENT NUMBER: 116:151788
TITLE: Preparation of pyrimidine derivatives as serotonin 2 receptor antagonists with high selectivity
INVENTOR(S): Watanabe, Yoshifumi; Kakui, Hiroyuki; Shibano, Toshiro
PATENT ASSIGNEE(S): Daiichi Seiyaku Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 18 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 03264579	A2	19911125	JP 1990-63910	19900314
JP 2860689	B2	19990224		

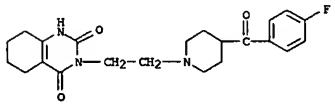
PRIORITY APPLN. INFO.: JP 1990-63910 19900314
OTHER SOURCE(S): MARPAT 116:151788
GI



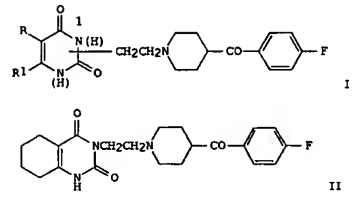
AB The title compds. [I; one of R1, R2 = H, alkyl, aralkyl and the other = Q, Q1; Z = linear or branched alkylene; R5, R6 = H, halo, alkyl, alkoxy; R7 = H, OH, alkyl, Ph; R3, R4 = H, alkyl, Ph, aralkyl; or R3R4 = C3-5 alkylene forming a 5- to 7-membered ring], useful as cardiovascular agents for treatment of ischemic heart disease and cerebral vascular disorders and for treatment of mental disorders such as depression or schizophrenia, are prepared Thus, 1.73 g EtO2CN:NCO2Et was added dropwise to a solution of 1-acetyl-5-phenyl-2,4(1H,3H)-pyrimidinedione preparation given 1.78. 2-[4-(4-Fluorobenzoyl)piperidin-1-yl]ethanol 2.15, and Ph3P 2.61 g in DMF with stirring under ice-cooling and the mixture was stirred for 2 h to give 14% I [R1 = R4 = R5 = R7 = H, R2 = Q, R3 = Ph, Z = (CH2)3, R6 = 4-F]. Serotonin 2 and α-1 receptor-antagonist activity with pA2 value of 7.7 and 6.6, resp. in rat's thoracic aorta contracted with serotonin.

IT **132332-47-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as serotoninergic S2 antagonist)

L4 ANSWER 34 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
RN 132332-47-9 HCAPLUS
CN 2,4(1H,3H)-Quinazolinedione, 3-[2-[4-(4-fluorobenzoyl)-1-piperidinyl]ethyl]-5,6,7,8-tetrahydro- (9CI) (CA INDEX NAME)



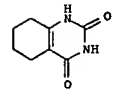
L4 ANSWER 35 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1991:549724 HCAPLUS
DOCUMENT NUMBER: 115:149724
TITLE: Syntheses of monocyclic and bicyclic 2,4(1H,3H)-pyrimidinediones and their serotonin 2 antagonist activities
AUTHOR(S): Watanabe, Yoshifumi; Usui, Hiroyuki; Shibano, Toshiro; Tanaka, Tsuyoshi; Kanao, Munefumi
CORPORATE SOURCE: Res. Inst., Daiichi Pharm. Co., Ltd., Tokyo, 134, Japan
SOURCE: Chemical & Pharmaceutical Bulletin (1990),.38(10), 2726-32
CODEN: CPBTAL; ISSN: 0009-2363
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 115:149724
GI



AB New serotonin 2 (5-HT2) antagonists with a monocyclic or bicyclic 2,4(1H,3H)-pyrimidinedione were prepared and their activities evaluated. In a series of monocyclic compds., I (1-substituted; R = Ph, R1 = H) showed potent in vitro activity, and the corresponding I (3-substituted derivs.; R = H, R1 = Ph; R = Ph, R1 = H; R = Ph, R1 = Me) also showed moderate activity. In the bicyclic compds., II exhibited the most potent activity among the compds. prepared The in vivo antagonist activity of II was comparable to that of ketanserin, a typical peripheral 5-HT2 antagonist. Structure-activity relationship is discussed.

IT **35042-48-9**
RL: RCT (Reactant); RACT (Reactant or reagent)
(alkylation of, with fluorobenzoylpiperidinyl ethanol by Mitsunobu reaction)

RN 35042-48-9 HCAPLUS
CN 2,4(1H,3H)-Quinazolinedione, 5,6,7,8-tetrahydro- (9CI) (CA INDEX NAME)



L4 ANSWER 35 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

L4 ANSWER 36 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1990:198956 HCAPLUS
DOCUMENT NUMBER: 112:198956
TITLE: A novel cyclization reaction of a C-6 substituted uridine analog: an entry to 5,6-dialkylated uridine derivatives
AUTHOR(S): Wang, Binghe; Kagel, John R.; Rao, T. S.; Mertes, Mathias P.
CORPORATE SOURCE: Dep. Med. Chem., Univ. Kansas, Lawrence, KS, 66045, USA
SOURCE: Tetrahedron Letters (1989), 30(50), 7005-8
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 112:198956

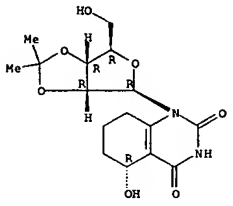
AB 5,6-Dialkylated uridine derivs. were conveniently synthesized in 5 steps starting from 2',3'-O-isopropylideneuridine in a 43% overall yield. The key reaction is a novel acid catalyzed cyclization of 6-(4-butanal)-2',3'-O-isopropylideneuridine.

IT 126740-11-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and dehydration of)

RN 126740-11-2 HCAPLUS

CN 2,4(1H,3H)-Quinazolinedione, 5,6,7,8-tetrahydro-5-hydroxy-1-[2,3-O-(1-methylethylidene)-β-D-ribofuranosyl]-, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 37 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN

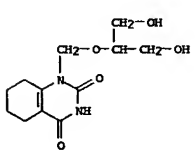
ACCESSION NUMBER: 1990:171858 HCAPLUS
DOCUMENT NUMBER: 112:171858
TITLE: Growth inhibition of Kirkman-Robbins hepatoma by 1-(1,3-dihydroxy-2-propoxymethyl)-5,6-tetramethyleneuracil and possible mechanism of its biological activity
AUTHOR(S): Greger, Janusz; Draminski, Marcin
CORPORATE SOURCE: Inst. Physiol. Biochem., Sch. Med., Lodz, 90131, Pol.
SOURCE: Zeitschrift fuer Naturforschung, C: Journal of Biosciences (1989), 44(11-12), 985-91
CODEN: ZNCBDA; ISSN: 0341-0382
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The effect of 1-(1,3-dihydroxy-2-propoxymethyl)-5,6-tetramethyleneuracil (DHPTU), an antitumor and antiviral acyclonucleoside, on Kirkman-Robbins hepatoma was studied in hamster. Tumor weight was reduced by 61% 48 h after i.p. administration of this drug (20 mg/kg). Inhibition of tumor growth was accompanied by a reduction of dThd, dGuo, and dTMP kinase activities in tumor cytosol (by 91%, 74% and 55%, resp.) and decrease in contents of dTTP, dGTP, and dATP (by 92%, 77%, and 67%, resp.) in dNTP pool. DHPTU was not phosphorylated by any tumor dN kinases, but was cleavage with TU release by the tumor cell enzyme, competitively inhibited by Formycin A (FA). After [14C]DHPTU or [14C]TU had been given i.p. to the animals with the tumor, 90% of the subcellular fraction labeling fell into the nuclear fraction. However, if [14C]DHPTU was administered with FA and deoxycoformycin (DCF), 27% of radioisotope was found in the nuclear fractions and 68% in cytosol. DCF prevented FA deamination to formycin B (FB) which is nt an inhibitor of the mentioned enzyme. DHPTU-induced changes in activity of dN kinases and dTMP kinase in hepatoma cells which may be attributed to the cytostatic activity of DHPTU seem to be connected to an enzyme which releases TU from DHPTU.

IT 110232-07-0
RL: BIOL (Biological study)
(deoxynucleoside kinase inhibition by, antihepatoma activity in relation to)

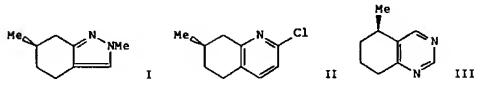
RN 110232-07-0 HCAPLUS

CN 2,4(1H,3H)-Quinazolinedione, 5,6,7,8-tetrahydro-1-[[2-hydroxy-1-(hydroxymethyl)ethoxy]methyl]- (9CI) (CA INDEX NAME)



L4 ANSWER 38 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1989:439307 HCAPLUS
DOCUMENT NUMBER: 111:39307
TITLE: Heterocyclic chemistry. VII. Synthesis of heterocycles from (+)-3-methylcyclohexanone
AUTHOR(S): Elguero, J.; Shimizu, B.
CORPORATE SOURCE: Inst. Quim. Med., CSIC, Madrid, 28006, Spain
SOURCE: Anales de Quimica, Serie C: Quimica Organica y Bioquimica (1988), 84(2), 176-82
CODEN: AQSBD6; ISSN: 0211-1357
DOCUMENT TYPE: Journal
LANGUAGE: French
OTHER SOURCE(S): CASREACT 111:39307
GI



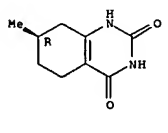
AB (+)-3-Methylcyclohexanone was prepared from pulegone and used to prepare a large family of tetramethyleneheterocycles: pyrazoles (4,5,6,7-tetrahydroindazoles, e.g., I), pyridines (5,6,7,8-tetrahydroquinolines, e.g., II), pyrimidines (5,6,7,8-tetrahydroquinazolines, e.g., III) pyridazines (5,6,7,8-tetrahydrocinnolines), pyrazines (5,6,7,8-tetrahydroquinoxalines and 1,2,3,4,5,6,7,8,9-octahydrophenazines) and quinoxalines (1,2,3,4-tetrahydrophenazines).

IT 121282-97-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and chlorination of, with phosphorus oxychloride)

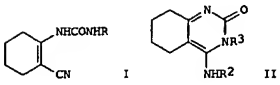
RN 121282-97-1 HCAPLUS

CN 2,4(1H,3H)-Quinazolinedione, 5,6,7,8-tetrahydro-7-methyl-, (R)- (9CI) (CA INDEX NAME)

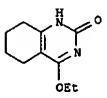
Absolute stereochemistry.



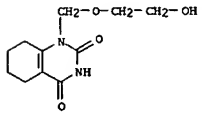
L4 ANSWER 39 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1989:95154 HCAPLUS
DOCUMENT NUMBER: 110:95154
TITLE: About the "Dimroth rearrangement" of aminohydroquinazolinones
AUTHOR(S): Bischoff, Christian; Schroeder, Edith
CORPORATE SOURCE: Zentralinst. Org. Chem., DAW, Berlin-Adlershof, Ger. Dem. Rep.
SOURCE: Journal fuer Praktische Chemie (Leipzig) (1988), 330(2), 289-92
CODEN: JPCEAO; ISSN: 0021-8383
DOCUMENT TYPE: Journal
LANGUAGE: German
OTHER SOURCE(S): CASREACT 110:95154
GI



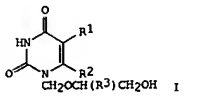
AB Reaction of urea I (R = H) with R1NH2.HCl (R1 = Ph, 2,6-Me2C6H3, 2,5-Me2C6H3) gave I (R = R1), whereas reaction with R1NH2 gave hexahydroquinazolinones II (R2 = H, R3 = R1) which rearranged to II (R2 = R1, R3 = H). These latter compds. were also obtained from 4-ethoxy-2,3,5,6,7,8-hexahydroquinazolin-2-one.
IT 98077-17-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with amines)
RN 98077-17-9 HCAPLUS
CN 2(1H)-Quinazolinone, 4-ethoxy-5,6,7,8-tetrahydro- (9CI) (CA INDEX NAME)



L4 ANSWER 40 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
RN 110232-05-8 HCAPLUS
CN 2,4(1H,3H)-Quinazolinedione, 5,6,7,8-tetrahydro-1-[(2-hydroxyethoxy)methyl]- (9CI) (CA INDEX NAME)

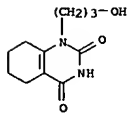


L4 ANSWER 40 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1988:124048 HCAPLUS
DOCUMENT NUMBER: 108:124048
TITLE: Inhibitor properties of some 5-substituted uracil acyclonucleosides, and 2,2'-anhydrouridines versus uridine phosphorylase from E. coli and mammalian sources
AUTHOR(S): Drabikowska, Alicja K.; Lissowska, Lidia; Veres, Zsuzsa; Shugar, David
CORPORATE SOURCE: Inst. Biochem. Biophys., Acad. Sci., Warsaw, 02-532, Pol.
SOURCE: Biochemical Pharmacology (1987), 36(23), 4125-8
CODEN: BCPCA6; ISSN: 0006-2952
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



AB Two series of 5-substituted uracil N(1)-acyclonucleosides [I, R1 = H, Me, Et, Pr, isoPr, CH2C6H5; R1R2 = (CH2)4; R3 = H, CH2OH] were examined as inhibitors of uridine phosphorylase from rat intestinal mucosa, and several I were also tested against the enzyme with Ehrlich ascites cells. In addition, several 5-substituted analogs of 2,2'-anhydrouridine were tested for their inhibitory effects vs. a highly purified uridine phosphorylase from Escherichia coli. The results were compared with published data for inhibition of the E. coli enzyme by the acyclonucleosides and of the rat enzyme by the anhydrouridines. In all instances, the inhibitors were active only vs. the uridine, but not thymidine, phosphorylase from E. coli, and inhibition was competitive with respect to uridine as substrate. In general, with 1 or 2 exceptions, inhibitory effects were more pronounced against the enzyme from mammalian sources. Amongst the acyclonucleoside analogs, the most effective inhibitor of the enzyme from the rat and Ehrlich ascites cells exhibited a Ki = 0.1 μM, comparable to that reported with the Sarcoma-180 enzyme, whereas the Ki for inhibition of the E. coli enzyme was 0.7 μM. By contrast, another effective inhibitor of the bacterial enzyme was 7-fold less potent against the mammalian enzyme. The 2,2'-anhydrouridines were 10-30-fold more effective against the rat, as compared to the E. coli, enzyme. The overall quant. data provide a reasonably good basis for the further design of potent inhibitors for possible use in chemotherapy.
IT 110232-05-8
RL: BIOL (Biological study)
(uridine phosphorylase inhibition by, in mammalian cells and Escherichia coli, structure in relation to)

L4 ANSWER 41 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1987:529717 HCAPLUS
DOCUMENT NUMBER: 107:129717
TITLE: Acyclonucleoside analogs consisting of 5- and 5,6-substituted uracils and different acylic chains: inhibitory properties vs purified E. coli uridine phosphorylase
AUTHOR(S): Drabikowska, Alicja K.; Lissowska, Lidia; Draminski, Marcin; Zgit-Wroblewska, Anna; Shugar, David
CORPORATE SOURCE: Inst. Biochem. Biophys., Warsaw, 02-532, Pol.
SOURCE: Zeitschrift fuer Naturforschung, C: Journal of Biosciences (1987), 42(3), 288-96
CODEN: ZNCBDA; ISSN: 0341-0382
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Synthetic procedures are described for the preparation of a variety of pyrimidine acyclonucleoside analogs, in which the aglycons are 5- and 5,6-substituted uracils, and the ribose moiety is replaced by different acyclic chains. These were examined as potential inhibitors of purified Escherichia coli uridine phosphorylase (I). None of the compds. was a substrate for I, or either a substrate or inhibitor of E. coli thymidine phosphorylase. Kinetic measurements were employed to determine Ki values for I inhibition. One of the more effective of these was 1-(1',3'-dihydroxy-2'-propoxy)methyl-5,6-tetramethyleneuracil (Ki = 2.7 μM). The same compound was a reasonably good inhibitor of the reverse, synthetic, reaction, with Ki values of 19 μM vs. uracil as the variable substrate, and 15 μM vs. α-D-ribose-1-phosphate as the variable substrate. For one of the analogs, racemic 1-(2',3'-dihydroxypropyl)-5,6-tetramethyleneuracil, it was shown that only the R-enantiomer was an inhibitor; the S-enantiomer was totally inactive. For several of the analogs, the corresponding isomeric N(3)-acyclonucleosides were inactive as inhibitors. The results for several of the good inhibitors were compared with those of other observers for inhibition of I from mammalian sources. Preliminary measurements with several of the analogs demonstrated that some of them were 1-2 orders of magnitude more effective against I from mammalian sources.
IT 72458-91-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and kinetics of Escherichia coli uridine phosphorylase inhibition by)
RN 72458-91-4 HCAPLUS
CN 2,4(1H,3H)-Quinazolinedione, 5,6,7,8-tetrahydro-1-(3-hydroxypropyl)- (9CI) (CA INDEX NAME)



L4 ANSWER 42 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1986:572393 HCAPLUS
DOCUMENT NUMBER: 105:172393
TITLE: Alkylated derivatives of uracil. Part X. Synthesis of 2,4-diketo-5,6,7,8-tetrahydroquinazoline
AUTHOR(S): Peczak, Grazyna; Draminski, Marcin
CORPORATE SOURCE: Inst. Basic Sci., Milit. Sch. Med., Lodz, 90647, Pol.
SOURCE: Polish Journal of Chemistry (1985), 59(3), 317-26
CODEN: PJCHDQ; ISSN: 0137-5083
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 105:172393
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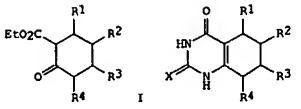
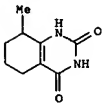


AB Refluxing esters I (R1, R2, R3, R4 = Me, H, H, Me2CH; Me2CH, H, H, Me; Me, H, H, H; H, Me, H, H; H, H, Me, H; H, H, H, Me) with thiourea 16 h in NaOEt-EtOH gave 32.6-75.0% quinazolines II (X = S) which were desulfurated by 10% aqueous ClCH2CO2H to give 62.6-87.0% II (X = O).
IT **63498-86-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 63498-86-2 HCAPLUS
CN 2,4(1H,3H)-Quinazolinedione, 5,6,7,8-tetrahydro-8-methyl- (9CI) (CA INDEX NAME)



L4 ANSWER 43 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1986:148828 HCAPLUS
DOCUMENT NUMBER: 104:148828
TITLE: 6-Alkyl- and 5,6-dialkyl-2-methoxy-4(3H)-pyrimidinones in the transformations of pyrimidines. Regiospecific 1-acylation of pyrimidines
AUTHOR(S): Botta, Maurizio; De Angelis, Francesco; Finizia, Gabriella; Nicoletti, Rosario; Delfini, Maurizio
CORPORATE SOURCE: Dip. Chim., Univ. "La Sapienza", Rome, 5-00185, Italy
SOURCE: Tetrahedron Letters (1985), 26(28), 3345-8
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 104:148828
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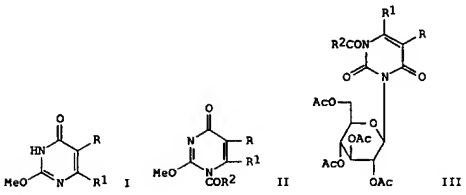
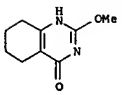
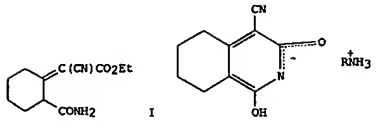


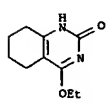
AB The 6- and 5,6-dialkyl-2-methoxy-4(3H)-pyrimidinones I [R = H, R1 = Me, RR1 = (CH2)4] were acylated to give 1-acylpyrimidine derivs. II [R2 = Ph, p-MeOC6H4 3,4-(methylenedioxy)phenyl] under Friedel-Craft-like conditions. In different acylation conditions 4-(acyloxy)pyrimidines were also obtained. II [R2 = 3,4-(methylenedioxy)phenyl] were converted into 1-acylisouridine analogs III.
IT **94815-67-5**
RL: RCT (Reactant); RACT (Reactant or reagent)
(silylation and Friedel-Crafts acylation of)
RN 94815-67-5 HCAPLUS
CN 4(1H)-Quinazolinone, 5,6,7,8-tetrahydro-2-methoxy- (9CI) (CA INDEX NAME)



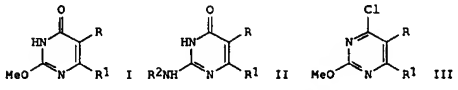
L4 ANSWER 44 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1985:523439 HCAPLUS
DOCUMENT NUMBER: 103:123439
TITLE: Formation of ethoxyhydroquinazolinone by attack of an ester carbonyl oxygen at a cyano group of an enamine
AUTHOR(S): Bischoff, Christian; Schroeder, Edith
CORPORATE SOURCE: Zentralinst. Org. Chem., Akad. Wiss. DDR, Berlin-Adlershof, DDR-1199, Ger. Dem. Rep.
SOURCE: Journal fuer Praktische Chemie (Leipzig) (1985), 327(1), 129-32
CODEN: JPCEAO; ISSN: 0021-8383
DOCUMENT TYPE: Journal
LANGUAGE: German
OTHER SOURCE(S): CASREACT 103:123439
GI



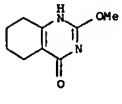
AB Et 2-oxocyclohexanecarboxylate was treated with H2NCN to give 4-ethoxy-2,3,5,6,7,8-hexahydroquinazolin-2-one. Bu 2-oxocyclopentanecarboxylate and H2NCN gave Bu 3-cyanaminocyclopent-1-enecarboxylate. 2-Oxocyclohexanecarboxamide reacted with EtO2CCH2CN and NaOH to give 4-cyanooctahydroisoquinoline-1,3-dione and with NH4OAc to give the Et cyclohexylidenecyanoacetate I. I was treated with NH3, H2NNH2, or cyclohexylamine to give the cyanohydroquinazolinedione salts II (R = H, NH2, cyclohexyl).
IT **98077-17-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrolysis of)
RN 98077-17-9 HCAPLUS
CN 2(1H)-Quinazolinone, 4-ethoxy-5,6,7,8-tetrahydro- (9CI) (CA INDEX NAME)



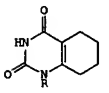
L4 ANSWER 45 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1985:422544 HCAPLUS
DOCUMENT NUMBER: 103:22544
TITLE: 6-Alkyl- and 5,6-dialkyl-2-methoxy-4-(3H)-pyrimidinones in the transformations of pyrimidines. Conversion into 2-substituted amino- and 4-chloropyrimidine derivatives
AUTHOR(S): Botta, M.; De Angelis, F.; Finizia, G.; Gambacorta, A.; Nicoletti, R.
CORPORATE SOURCE: Dep. Chem., Univ. "La Sapienza", Rome, 00185, Italy
SOURCE: Synthetic Communications (1985), 15(1), 27-34
CODEN: SYNCAV; ISSN: 0039-7911
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 103:22544
GI



AB Pyrimidinones I [R = H, Me; R1 = Me, or RR1 = (CH2)4] were converted to amino analogs II (R2 = Bu, cyclohexyl, Ph), and chloropyrimidines III were obtained from I and SOCl2. I (R = H, R1 = Me) was treated with NaH and BuNH2 in tetralin to give II (R = H, R1 = Me, R2 = Bu).
IT **94815-67-5**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reactions of, with amines and thionyl chloride)
RN 94815-67-5 HCAPLUS
CN 4(1H)-Quinazolinone, 5,6,7,8-tetrahydro-2-methoxy- (9CI) (CA INDEX NAME)



L4 ANSWER 46 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1985:185410 HCAPLUS
DOCUMENT NUMBER: 102:185410
TITLE: Structural analogs of 5,6-tetramethyleneuracil ribosides - inhibitors of enzymes participating in nucleic acid synthesis
AUTHOR(S): Draminski, Marcin; Frass, Elzbieta; Greger, Janusz; Fabianowska-Majewska, Krystyna
CORPORATE SOURCE: Inst. Physiol. Biochem., Mil. Sch. Med., Lodz, 906 47, Pol.
SOURCE: Collection of Czechoslovak Chemical Communications (1985), 50(1), 280-5
CODEN: CCCCAK; ISSN: 0366-547X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 102:185410
GI

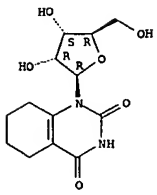


I

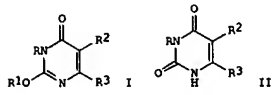
AB N-1 and N-3 ribosyl, allyl, and (RS)-2,3-dihydroxypropyl derivs. of 5,6-tetramethyleneuracil were prepared, e.g., allylation of 2,4-bis(O-trimethylsilyl)-5,6-tetramethyleneuracil with allyl bromide at 90-100° for 20 h gave 75% allyl derivative (I, R = allyl), which was treated with NaClO3 and OsO4 in MeOH-H2O at room temperature overnight to give 45% dihydroxypropyl derivative [I, R = CH2CH(OH)CH2OH]]. Some of the compds. prepared are inhibitors of enzymes involved in regulation of DNA synthesis.
IT 75252-32-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and deoxynucleoside kinase inhibition by)
RN 75252-32-3 HCAPLUS
CN 2,4(1H,3H)-Quinazolinedione, 5,6,7,8-tetrahydro-1-β-D-ribofuranosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 46 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

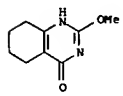


L4 ANSWER 47 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1985:78816 HCAPLUS
DOCUMENT NUMBER: 102:78816
TITLE: 6-Alkyl and 5,6-dialkyl-2-methoxy-4(3H)-pyrimidinones in the transformations of pyrimidines - 2. Synthesis and conversion into alkyluracils and 2-alkoxy-4(3H)-pyrimidinones
AUTHOR(S): Botta, M.; Cavalieri, M.; Ceci, D.; De Angelis, F.; Finizia, G.; Nicoletti, R.
CORPORATE SOURCE: Dep. Chem., Univ. "La Sapienza", Rome, 00185, Italy
SOURCE: Tetrahedron (1984), 40(17), 3313-20
CODEN: TETRAB; ISSN: 0040-4020
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 102:78816
GI

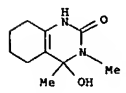


I II

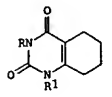
AB Alkoxypyrimidinones I [R = H; R1 = Me; R2 = H, R3 = Me, Et; R2 = R3 = Me; R2R3 = (CH2)4] were obtained by treating R3COCHR2CO2Et with MeOC(NH2):NH.H2SO4 and Ca(OH)2. Similar reaction, followed by acidification, gave pyrimidinediones II [R = H; R2 = H, Me, allyl, octyl; R3 = Me, Et, pentyl, cyclohexyl; R2R3 = (CH2)4]. I (R1 = Et, Bu, cyclohexyl) were prepared by transalkylation of I (R1 = Me) with alcoholate. I (R = H, R1 = Me) and II (R = H) were N-methylated with Me2SO4 to give I and II (R = Me).
IT 94815-67-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and transalkylation of)
RN 94815-67-5 HCAPLUS
CN 4(1H)-Quinazolinone, 5,6,7,8-tetrahydro-2-methoxy- (9CI) (CA INDEX NAME)



L4 ANSWER 48 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1985:19808 HCAPLUS
DOCUMENT NUMBER: 102:19808
TITLE: Sublimation heat in alkyl derivatives of nucleic acid bases
AUTHOR(S): Glukhova, O. T.
CORPORATE SOURCE: Inst. Low Temp. Phys. Eng., Kharkov, USSR
SOURCE: Studia Biophysica (1984), 101, 25-6
CODEN: STBIBN; ISSN: 0081-6337
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The heat of sublimation (ΔHs) of cytosine, uracil, thymine, adenine, and their alkyl derivs. was calculated from the temperature dependence of their evaporation rates (determined by the low-temperature quartz-resonator method of O. T. Glukhora, et al., 1982). The substitution of Me groups at H-bonding sites results in decreased ΔHs values for pyrimidine bases. The smaller decrease in ΔHs values for adenine derivs. may be due to the high contribution of stacking interaction to the ΔHs of purines as compared to pyrimidine bases.
IT 93824-16-9
RL: PRP (Properties)
(heat of sublimation of)
RN 93824-16-9 HCAPLUS
CN 2(1H)-Quinazolinone, 3,4,5,6,7,8-hexahydro-4-hydroxy-3,4-dimethyl- (9CI) (CA INDEX NAME)

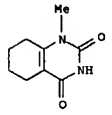


L4 ANSWER 49 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1983:179812 HCAPLUS
DOCUMENT NUMBER: 98:179812
TITLE: Alkylated derivatives of uracil. Part IX. Syntheses of N-(2,3-dihydroxypropyl) derivatives of 5,6-tetramethyleneuracil, structural analogs of nucleosides
AUTHOR(S): Draminski, Marcin; Frass, Elzbieta
CORPORATE SOURCE: Inst. Physiol. Biochem., Mil. Sch. Med., Lodz, 90647, Pol.
SOURCE: Polish Journal of Chemistry (1981), 55(7-8), 1547-52
CODEN: PJCHDQ; ISSN: 0137-5083
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



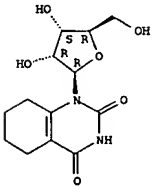
I

AB Tetramethyleneuracils I [one of R and R1 is H and the other is Me, CH2:CHCH2, HOCH2CH(OH)CH2, D-ribofuranosyl] were prepared and their UV, mass, and NMR spectra determined Thus, 5,6-tetramethyleneuracil was silylated with Me3SiCl and the resultant 2,4-di-O-trimethylsilyl derivative was methylated with MeI in C6H6 in the presence of AgClO4 to give I (R = H, R1 = Me). Cyclocondensation of 2-carbethoxycyclohexanone with MeNHCSNH2 gave 3-N-methyl-5,6-tetramethylene-2-thiouracil, which on refluxing with ClCH2CO2H gave I (R = Me, R1 = H).
IT 33738-24-8P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and spectra of)
RN 33738-24-8 HCAPLUS
CN 2,4(1H,3H)-Quinazolinedione, 5,6,7,8-tetrahydro-1-methyl- (8CI, 9CI) (CA INDEX NAME)

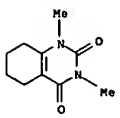


L4 ANSWER 50 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1982:451653 HCAPLUS
DOCUMENT NUMBER: 97:51653
TITLE: Pyrimidine ribonucleoside phosphorylase activity vs. 5- and/or 6-substituted uracil and uridine analogs, including conformational aspects
AUTHOR(S): Krajewska, Estera; Shugar, David
CORPORATE SOURCE: Inst. Biochem. Biophys., Acad. Sci., Warsaw, 02-532, Pol.
SOURCE: Biochemical Pharmacology (1982), 31(6), 1097-102
CODEN: BCPCA6; ISSN: 0006-2952
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The relative rates of formation (from α-D-ribose-1-phosphate and the appropriate base) and phosphorylysis of various uracil/uridine analogs by Salmonella typhimurium pyrimidine nucleoside phosphorylase (EC 2.4.2.1) were investigated. The Km and Vmax values of the phosphorolysis of 5- and(or) 6-substituted uridines are given. The results are discussed in relation to pyrimidine structure and conformation.
IT 75252-32-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with pyrimidine nucleoside phosphorylase of Salmonella, kinetics of, structure and conformation in relation to)
RN 75252-32-3 HCAPLUS
CN 2,4(1H,3H)-Quinazolinedione, 5,6,7,8-tetrahydro-1-β-D-ribofuranosyl- (9CI) (CA INDEX NAME)

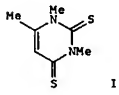
Absolute stereochemistry.



L4 ANSWER 51 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1982:451335 HCAPLUS
DOCUMENT NUMBER: 97:51335
TITLE: Thermochemistry of aqueous solutions of alkylated nucleic acid bases. IV. Enthalpies of hydration of 5-alkyluracils
AUTHOR(S): Teplitskii, A. B.; Glukhova, O. T.; Sukhodub, L. F.; Yanson, I. K.; Zielenkiewicz, A.; Zielenkiewicz, W.; Kosinski, J.; Wierzchowski, K. L.
CORPORATE SOURCE: Phys.-Tech. Inst. Low Temp., Kharkov, 310164, USSR
SOURCE: Biophysical Chemistry (1982), 15(2), 139-47
CODEN: BICIAZ; ISSN: 0301-4622
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Enthalpies of sublimation, ΔH0subl, and of solution in water, ΔH0sol, were determined for a series of crystalline 1,3-dimethyluracil derivs. substituted at the C5-ring C atom with alkyl groups (-CnH2n+1, n = 2-4) and some of their C5,6-cyclooligomethylene analogs (-(CH2)n-, n = 3-5). From these data, enthalpies of hydration ΔH0hydr = ΔH0sol - ΔH0subl, were calculated and corrected for energies of cavity formation in pure liquid water to obtain enthalpies of interaction, ΔH0int, of the solutes with their hydration shells. The latter are discussed together with the recalcd. ΔH0int for variously methylated uracils, obtained previously according to a simplified correction procedure, in terms of perturbations in the energy and scheme of hydration of the diketopyrimidine ring brought about by alkyl substitution. Each CH2 group added with an alkyl substitution contributes favorably .apprx.-20 kJ/mol to ΔH0int. This contribution is partially canceled by the unfavorable contribution to H0int connected with removal of some water mols. bound in the 1st and subsequent hydration layers by an alkyl substituent. This is particularly evident on substitution at the polar side of the diketopyrimidine ring on which water mols. are expected to be bound specifically.
IT 80254-48-4
RL: PRP (Properties)
(heat of hydration of)
RN 80254-48-4 HCAPLUS
CN 2,4(1H,3H)-Quinazolinedione, 5,6,7,8-tetrahydro-1,3-dimethyl- (9CI) (CA INDEX NAME)

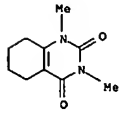


L4 ANSWER 52 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1982:35183 HCAPLUS
DOCUMENT NUMBER: 96:35183
TITLE: 1,2,3,4-Tetrahydropyrimidine- and 1,2,3,4,5,6,7,8-octahydroquinazoline-2,4-dithiones and 2,4-diones. Synthesis and mechanistic study
AUTHOR(S): Lamazouere, A. M.; Sotiropoulos, J.
CORPORATE SOURCE: Lab. Chim. Org. Appl., Univ. Paul Sabatier, Toulouse, 31062, Fr.
SOURCE: Tetrahedron (1981), 37(14), 2451-7
CODEN: TETRAB; ISSN: 0040-4020
DOCUMENT TYPE: Journal
LANGUAGE: French
OTHER SOURCE(S): CASREACT 96:35183
GI

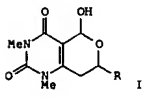


I

AB Tetrahydropyrimidinedithiones and octahydroquinazolinedithiones were prepared by cycloaddn. reactions in basic medium of alkyl or aryl isothiocyanates with ketones having ≥1 α-H. E. g., reaction of Me2CO with MeNCS (EtCMe2ONa, C6H6, inert atmospheric, 0°, 15 h) gave 32% pyrimidine I. The complex mechanism of this reaction was studied. Desulfurization of the dithiones by refluxing with Hg(OAc)2-AcOH (Me2CO, 2 h) gave the corresponding diketones.
IT 80254-48-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 80254-48-4 HCAPLUS
CN 2,4(1H,3H)-Quinazolinedione, 5,6,7,8-tetrahydro-1,3-dimethyl- (9CI) (CA INDEX NAME)

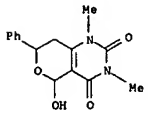


L4 ANSWER 53 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1981:121457 HCAPLUS
DOCUMENT NUMBER: 94:121457
TITLE: Cycloaddition reaction of 5-formyl-1,3,6-trimethyluracil with aldehydes. New synthetic approach to pyrano[4,3-d]pyrimidines
AUTHOR(S): Hirota, Kosaku; Asao, Tetsuji; Sugiyama, Isao; Senda, Shigeo
CORPORATE SOURCE: Gifu Coll. Pharm., Gifu, 502, Japan
SOURCE: Heterocycles (1981), 15(1), 289-92
CODEN: HTCYAM; ISSN: 0385-5414
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 94:121457
GI

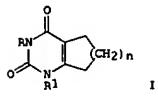


I

AB Pyranopyrimidines I (R = H, Et, Ph, CH2Ph, 2-furyl, 1,3,6-trimethyluracil-5-yl) were obtained in 13-88% yield by treating 5-formyl-1,3,6-trimethyluracil with RCHO and LiN(CHMe2)2. I (R = Ph) was converted to its Me ether or was cleaved with SOCl2 to 5-formyl-1,3-dimethyl-6-styryluracil, which was deformylated with acid.
IT 76952-30-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reactions of)
RN 76952-30-2 HCAPLUS
CN 2H-Pyrano[4,3-d]pyrimidine-2,4(3H)-dione, 1,5,7,8-tetrahydro-5-hydroxy-1,3-dimethyl-7-phenyl- (9CI) (CA INDEX NAME)



L4 ANSWER 54 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1980:586714 HCAPLUS
DOCUMENT NUMBER: 93:186714
TITLE: Alkylated derivatives of uracil. Part VIII. Synthesis of 5,6-oligomethyleneuracil ribosides - potential antimetabolites
AUTHOR(S): Frass, Elzbieta; Draminski, Marcin
CORPORATE SOURCE: Inst. Physiol. Biochem., Mil. Sch. Med., Lodz, 90647, Pol.
SOURCE: Polish Journal of Chemistry (1980), 54(2), 189-93
CODEN: PJCHDQ; ISSN: 0137-5083
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

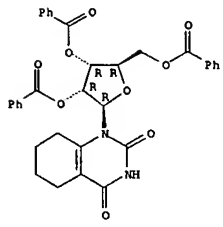


I

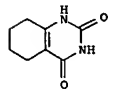
AB β-Nucleosides I (R = H, R1 = ribosyl, n = 1, 2, 3; R = ribosyl, R1 = H, n = 1, 2, 3) were prepared by glycosylation of trimethylsilylated 5,6-(oligomethylene)uracils with 1-O-acetyl- or 1-chloro-2,3,5-tri-O-benzoylribofuranose, followed by debenzoylation. I (R = ribosyl, R1 = H, n = 2) was an effective inhibitor of thymidine kinase and thymidylate kinase.
IT 75252-25-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and debenzoylation of)
RN 75252-25-4 HCAPLUS
CN 2,4(1H,3H)-Quinazolinedione, 5,6,7,8-tetrahydro-1-(2,3,5-tri-O-benzoyl-β-D-ribofuranosyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

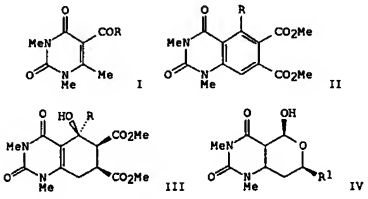
L4 ANSWER 54 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



L4 ANSWER 55 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1980:585255 HCAPLUS
DOCUMENT NUMBER: 93:185255
TITLE: Behavior of N-allyl-5,6-tetramethyleneuracils under electron impact
AUTHOR(S): Draminski, M.
CORPORATE SOURCE: Physiol.-Biochem. Inst., Mil.-Med. Acad., Lodz, Pol.
SOURCE: Khimiya Geterotsiklicheskikh Soedinenii (1980), (5), 705
CODEN: KGSSAQ; ISSN: 0453-8234
DOCUMENT TYPE: Journal
LANGUAGE: Russian
AB The [M-15]+ peak in the mass spectra of the title compds. resulted from cleavage of the alicyclic ring with H migration to form a Me group, which was then lost.
IT 35042-48-9
RL: PRP (Properties)
(mass spectrum of)
RN 35042-48-9 HCAPLUS
CN 2,4(1H,3H)-Quinazolinedione, 5,6,7,8-tetrahydro- (9CI) (CA INDEX NAME)



L4 ANSWER 56 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1980:471698 HCAPLUS
DOCUMENT NUMBER: 93:71698
TITLE: Cycloaddition reaction of a pyrimidine dienol
AUTHOR(S): Senda, Shigeo; Hirato, Kosaku; Asao, Tetsuji; Sugiyama, Isao
CORPORATE SOURCE: Gifu Coll. Pharm., Higashi, 502, Japan
SOURCE: Fukusokan Kagaku Toronkai Koen Yoshishu, 12th (1979), 261-5. Kitasato Daigaku Yakugakubu: Tokyo, Japan. CODEN: 42VCA9
DOCUMENT TYPE: Conference
LANGUAGE: Japanese
GI



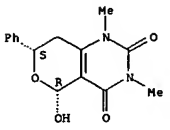
AB Pyrimidinediones I (R = H, Me, EtO) underwent base-catalyzed isomerization and Diels-Alder reactions with dienophiles and aldehydes. Thus, isomerization of I with (Me2CH)2NLi and subsequent cyclization-oxidation with MeO2CC.tplbond.CCO2Me gave quinazolines II, and isomerization-cyclization of I (R = H, Me) with di-Me maleate gave quinazolines III. Isomerization-cyclization of I (R = H) with R1CHO (R1 = H, Et, Ph, PhCH2, furfuryl) gave pyranopyrimidines IV.

IT **74301-67-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reactions of)

RN 74301-67-0 HCAPLUS
CN 2H-Pyrano[4,3-d]pyrimidine-2,4(3H)-dione, 1,5,7,8-tetrahydro-5-hydroxy-1,3-dimethyl-7-phenyl-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.

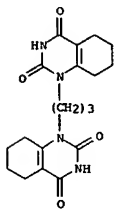
L4 ANSWER 56 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



L4 ANSWER 57 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1980:471684 HCAPLUS
DOCUMENT NUMBER: 93:71684
TITLE: Physical and photochemical properties of 1,1'-trimethylenebis(5,6-oligomethylene)uracils
AUTHOR(S): Golankiewicz, Krzysztof; Celewicz, Lech
CORPORATE SOURCE: Inst. Chem., Adam Mickiewicz Univ., Poznan, 60780, Pol.
SOURCE: Polish Journal of Chemistry (1979), 53(10), 2075-81 CODEN: PJCHDQ; ISSN: 0137-5083
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB The title compds. I (m = 3,4; n = 0, 3, 4) and related compds. were irradiated by UV light to give photodimers at varying rates. Dimerization of I (m = n = 4) was particularly slow, which is explained by the steric bulk of the 2 cyclohexene systems and the hindering of non-bonded base-base interactions. The photochem. reversibility of the photodimers indicates a cyclobutane-type structure, e.g., II, which reacted with C6H4(CH2Br)2-o to give xylylene derivs. e.g., III.

IT **67603-05-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and photodimerization of)

RN 67603-05-8 HCAPLUS
CN 2,4(1H,3H)-Quinazolinedione, 1,1'-(1,3-propanediyl)bis[5,6,7,8-tetrahydro- (9CI) (CA INDEX NAME)



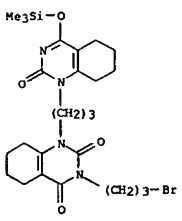
L4 ANSWER 58 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1980:58714 HCAPLUS
DOCUMENT NUMBER: 92:58714
TITLE: By-products of ω-bromoalkylation reaction of trimethylsilyl derivatives of uracil
AUTHOR(S): Golankiewicz, Krzysztof; Celewicz, Lech
CORPORATE SOURCE: Inst. Chem., Adam Mickiewicz Univ., Poznan, 60780, Pol.
SOURCE: Polish Journal of Chemistry (1979), 53(6), 1367-71 CODEN: PJCHDQ; ISSN: 0137-5083
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 92:58714
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

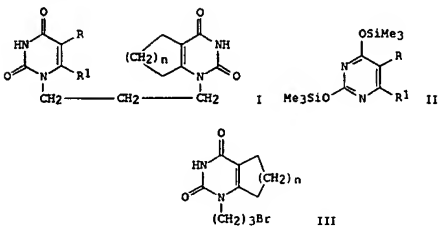
AB Bromopropylation of uracil derivs. (I; n = 1, 2) gave the desired bis(3-bromopropyl) derivs. II as well as coupling by-products III and IV. The hydroxypropyl derivs. (V) were obtained by hydrolysis of the ring-closure intermediates VI.

IT **72458-90-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and bromopropylation of)

RN 72458-90-3 HCAPLUS
CN 2,4(1H,3H)-Quinazolinedione, 3-(3-bromopropyl)-5,6,7,8-tetrahydro-1-[3-[5,6,7,8-tetrahydro-2-oxo-4-[(trimethylsilyl)oxy]-1(2H)-quinazolinyl]propyl]- (9CI) (CA INDEX NAME)

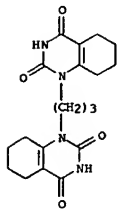


L4 ANSWER 59 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1978:529475 HCAPLUS
DOCUMENT NUMBER: 89:129475
TITLE: Synthesis of new derivatives of 1,1'-trimethylenebispyrimidines
AUTHOR(S): Golankiewicz, Krzysztof; Celewicz, Lech
CORPORATE SOURCE: Inst. Chem., Adam Mickiewicz Univ., Poznan, Pol.
SOURCE: Polish Journal of Chemistry (1978), 52(5), 1035-8
CODEN: PJCHDQ; ISSN: 0137-5083
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

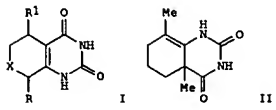


AB Seven trimethylenebispyrimidines I [R = H, Me, R1 = H, n = 1,2; (RR1) = (CH2)3, (CH2)4, n = 1,2] were prepared in 30-54% yield by heating silylated uracils II with (bromopropyl)uracils III in EtOH-CHCl3.
IT **67603-05-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 67603-05-8 HCAPLUS
CN 2,4(1H,3H)-Quinazolinedione, 1,1'-(1,3-propanediyl)bis[5,6,7,8-tetrahydro- (9CI) (CA INDEX NAME)

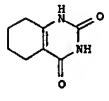
L4 ANSWER 59 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



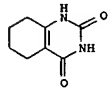
L4 ANSWER 60 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1977:468278 HCAPLUS
DOCUMENT NUMBER: 87:68278
TITLE: Synthesis of pyrimidine-2,4-diones from ketones and urea
AUTHOR(S): Bischoff, Christian; Herma, Hannelore; Schroeder, Edith
CORPORATE SOURCE: Zentralinst. Org. Chem., DAW, Berlin-Adlershof, Ger. Dem. Rep.
SOURCE: Journal fuer Praktische Chemie (Leipzig) (1977), 319(2), 230-4
CODEN: JPCEAO; ISSN: 0021-8383
DOCUMENT TYPE: Journal
LANGUAGE: German
OTHER SOURCE(S): CASREACT 87:68278
GI



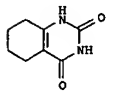
AB Pyrimidinediones I (X = CH2, R = (CH2)nMe, cyclohexyl, R1 = H, n = 0-7; X = CH2, R = CHMe2, R1 = Me; X = CHPh, R = H, R1 = Ph; X = (CH2)3,7, R = R1 = H) were prepared by condensing ketones with urea in the presence of p-MeC6H4SO3H. Reaction of 2,5-dimethylcyclohexanone with urea gave II.
IT **35042-48-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 35042-48-9 HCAPLUS
CN 2,4(1H,3H)-Quinazolinedione, 5,6,7,8-tetrahydro- (9CI) (CA INDEX NAME)



L4 ANSWER 61 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1974:569505 HCAPLUS
DOCUMENT NUMBER: 81:169505
TITLE: Alkylated derivatives of uracil. VI. Synthesis and properties of 5,6-oligomethyleneuracils
AUTHOR(S): Fraas, Elzbieta; Draminski, Marcin; Fiszer, Bernard
CORPORATE SOURCE: Dep. Gen. Physiol. Chem., Mil. Sch. Med., Lodz, Pol.
SOURCE: Roczniki Chemii (1974), 48(6), 971-80
CODEN: ROCHAC; ISSN: 0035-7677
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB Reaction of β-keto esters and thiourea gave I (n = 1, 2, 3; X = S) and II (R = Me, Et; R1 = Me, Et, Pr; X = S) I (X = S) were converted to I (X = O) by heating with 10% ClCH2CO2H. Irradiation of I and II with a low pressure lamp gave only 10% yields of products.
IT **35042-48-9P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and spectra of)
RN 35042-48-9 HCAPLUS
CN 2,4(1H,3H)-Quinazolinedione, 5,6,7,8-tetrahydro- (9CI) (CA INDEX NAME)



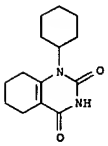
L4 ANSWER 62 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1974:520567 HCAPLUS
DOCUMENT NUMBER: 81:120567
TITLE: Pyrimidines and condensed derivatives. III. Synthesis of some isocytosines and related imidazo[1,2-a]- and [1,2-c]pyrimidinones
AUTHOR(S): Agai, Bela; Hornyak, Gyula; Lempert, Karoly
CORPORATE SOURCE: Dep. Org. Chem., Tech. Univ. Budapest, Budapest, Hung.
SOURCE: Periodica Polytechnica, Chemical Engineering (1974), 18(1), 47-72
CODEN: PDPTAE; ISSN: 0324-5853
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Isocytosines I-III [R = CH2CH2OH, (CH2)3OH, CH2CO2H, Bu, CH2Ph, R1 = H; RR1 = (CH2)3-4; R2 = H, Me, Et; R3 = H,allyl; R4 = Me, 2-butenyl, CH2CH2CO2H; R3R4 = (CH2)3-4] were prepared by aminolysis of the corresponding methylthio compds., obtained by methylating appropriate thiouracils. I-III (R = CH2CH2OH) were chlorinated and cyclized to imid-azopyrimidinones.
IT **35042-48-9**
RL: RCT (Reactant); RACT (Reactant or reagent)
(sulfurization of)
RN 35042-48-9 HCAPLUS
CN 2,4(1H,3H)-Quinazolinedione, 5,6,7,8-tetrahydro- (9CI) (CA INDEX NAME)



L4 ANSWER 63 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1973:438704 HCAPLUS
DOCUMENT NUMBER: 79:38704
TITLE: Hpynotic uracil derivatives
INVENTOR(S): Ley, Kurt; Aichinger, Gerd; Hagemann, Hermann; Niemers, Ekkehard; Hoffmeister, Friedrich
PATENT ASSIGNEE(S): Bayer A.-G.
SOURCE: Ger. Offen., 28 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2142317	A1	19730301	DE 1971-2142317	19710824
PRIORITY APPLN. INFO.:			DE 1971-2142317 A	19710824

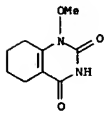
AB The reaction of N-chlorocarbonyl isocyanate [27738-96-1] with the appropriate acetophenone, imine, oxime, and (or) hydrazone yielded uracil derivs. (I; R = alkyl, alkenyl, cycloalkyl, aralkyl, aryl, alkoxyalkyl, alkoxy, aralkoxy, dialkylaminoalkoxy, dialkylamino, dialkenylamino, or morpholino; R1 = H, alkyl, alkenyl, dialkylaminoalkyl, or aralkyl; R2 = H, alkyl, aryl, or halogen; and R3 = alkyl, alkenyl, cycloalkyl, aralkyl, aralkenyl, or aryl), which demonstrated potent hypnotic properties in mice and rabbits. Thus, ClCONCO was treated with the ketimine from acetophenone and p-chloroaniline in PhCl at 30-5.deg., to give 1-(4-chlorophenyl)-6-phenyluracil (I; R = 4-ClC6H4, R1 = R2 = H, R3 = Ph) (II) [40771-57-1]. II had an oral LD50 of 616 mg/kg in mice; inhibited the orientation motility and the righting reflex at 16.5 and 445 mg/kg (oral) resp.; had a narcosis index of 3.3 (based on the inhibition of the righting reflex and motility); and had a hypnotic action at 4 mg/kg (oral) in rabbits (based on the dose which increased the electroencephalographic sleep by 50%). The action of these newly synthesized compds. was compared with the standard hypnotics, methyprylon and cyclobarbital.
IT **33443-60-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 33443-60-6 HCAPLUS
CN 2,4(1H,3H)-Quinazolinedione, 1-cyclohexyl-5,6,7,8-tetrahydro- (8CI, 9CI) (CA INDEX NAME)



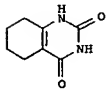
L4 ANSWER 64 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1973:111360 HCAPLUS
DOCUMENT NUMBER: 78:111360
TITLE: Uracil derivatives
INVENTOR(S): Ley, Kurt; Aichinger, Gerd; Botta, Arthur; Hagemann, Hermann; Niemers, Ekkehard
PATENT ASSIGNEE(S): Farbenfabriken Bayer A.-G.
SOURCE: Ger. Offen., 18 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2126148	A	19721207	DE 1971-2126148	19710526
PRIORITY APPLN. INFO.:			DE 1971-2126148	19710526

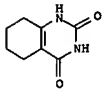
GI For diagram(s), see printed CA Issue.
AB Thirty-nine uracil derivs. of the general formula I, e.g. I [R = OCH2Ph, morpholino; R1 = Ph, Cl, OMe; R2 = H; RR2 = (CH2)10], II (n = 2, 4; m = 2, 3), or III, were prepared by reaction of R2CH2C(:NR)R1 with XCONCO (X = Cl, PhO) or (EtO2C)2NH and were useful as plant protective agents. Thus, melting 1,8-diazabicyclo[5.3.0]dec-7-ene and (EtO2C)2NH and distillation of EtOH gave 62.9% II (n = 4, m = 2).
IT **40721-46-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 40721-46-8 HCAPLUS
CN 2,4(1H,3H)-Quinazolinedione, 5,6,7,8-tetrahydro-1-methoxy- (9CI) (CA INDEX NAME)



L4 ANSWER 65 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1972:539566 HCAPLUS
DOCUMENT NUMBER: 77:139566
TITLE: Synthesis of β-cyano-α,β-unsaturated isocyanates and their reactions with hydrogen chloride
AUTHOR(S): Ohoka, Masataka; Yanagida, Shozo; Komori, Saburo
CORPORATE SOURCE: Fac. Eng., Osaka Univ., Suita, Japan
SOURCE: Journal of Organic Chemistry (1972), 37(19), 3030-2
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
AB When enaminonitriles with a primary N atom were treated with phosgene in refluxing EtOAc, N-acylation occurred to give the corresponding β-cyano-α,β-unsatd. isocyanates in 37-79% yield. The reaction of thus obtained isocyanates with HCl in dioxane at 100° 24 hr gave 5,6-disubstituted uracils in good yields. Reaction of (Z)-2-cyano-1-phenylpropenyl isocyanate with HCl at 60° 6 hr afforded 6-chloro-5-methyl-4-phenyl-2(3H)-pyrimidinone.
IT **35042-48-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 35042-48-9 HCAPLUS
CN 2,4(1H,3H)-Quinazolinedione, 5,6,7,8-tetrahydro- (9CI) (CA INDEX NAME)



L4 ANSWER 66 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1972:461940 HCAPLUS
DOCUMENT NUMBER: 77:61940
TITLE: Catalytic condensation of dicyandiamide with cyclohexanone
AUTHOR(S): Vodop'yanov, V. G.; Golov, V. G.; Mushkin, Yu. I.
CORPORATE SOURCE: Gos. Nauchno-Issled. Proekt. Inst. Azotn. Prom. Khim. Prod. Org., Dzerzhinsk, USSR
SOURCE: Zhurnal Organicheskoi Khimii (1972), 8(5), 1000-3
CODEN: ZORKAE; ISSN: 0514-7492
DOCUMENT TYPE: Journal
LANGUAGE: Russian
GI For diagram(s), see printed CA Issue.
AB Condensation of (H2N)2C:NCN with cyclohexanone in the presence of Et3N yielded 67.4% 2,4-diamino-5,6-cyclohexenopyrimidine (I); in the presence of NaOH or NaOEt, 39.4% RNH[C(NH2):N]2CN (II, R = 1-cyclohexenyl) was formed. Treatment of II with 20% H2SO4 afforded H2SO4.-(H2N)2C:NCONHCONH2, which gave ammelide with refluxing aqueous NaOH. Heating with 55% H2SO4 yielded 2-amino-4-oxo-5,6-cyclohexeno-3,4-dihydropyrimidine, dihydropyrimidine, which was diazotized to give 2,4-dioxo-5,6-cyclohexeno-1,2,3,4-tetrahydropyrimidine.
IT **35042-48-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 35042-48-9 HCAPLUS
CN 2,4(1H,3H)-Quinazolinedione, 5,6,7,8-tetrahydro- (9CI) (CA INDEX NAME)

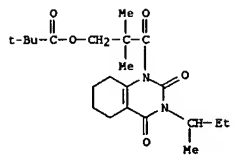


L4 ANSWER 67 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1972:419672 HCAPLUS
DOCUMENT NUMBER: 77:19672
TITLE: Herbicidal 1-pivaloyluracils
INVENTOR(S): Zeidler, Adolf; Kiefer, Hans; Fischer, Adolf; Hoffmann, Hans Dieter; Merger, Franz
PATENT ASSIGNEE(S): Badische Anilin- & Soda-Fabrik AG
SOURCE: Ger. Offen., 13 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2041996	A	19720316	DE 1970-2041996	19700825
US 3758477	A	19730911	US 1971-167844	19710730
AU 7132126	A1	19730215	AU 1971-32126	19710809
ZA 7105366	A	19720531	ZA 1971-5366	19710811
SU 390696	D	19730711	SU 1971-1691734	19710820
HU 162722	P	19730428	HU 1971-BA2637	19710823
BE 771695	A1	19720224	BE 1971-107373	19710824
NL 7111627	A	19720229	NL 1971-11627	19710824
AT 309885	B	19730910	AT 1971-7395	19710824
FR 2106030	A5	19720428	FR 1971-30852	19710825
GB 1352255	A	19740508	GB 1971-39781	19710825

PRIORITY APPLN. INFO.: DE 1970-2041996 A 19700825
GI For diagram(s), see printed CA Issue.
AB Ten title compds. I, R = ClCH2CO2CH2CMe2CO = R4, AcOCH2CMe2CO, EtCHMeCO, or BrCH2CMe2CO; R1 = iso-Pr, sec-Bu, or cyclohexyl; R2 = Br; R3 = Me; or R2R3 = (CH2)3 or (CH2)4 were prepared by reaction of I (R = H) with chlorides RCl. (CH2)4 Thus, 241 parts 3-isopropyl-5-bromo-6-methyluracil was treated with R4Cl in PhMe in the presence of Et3N for 3.5 hr at 80° to give 220 parts I (R = R4, R1 = iso-Pr, R2 = Br, R3 = Me) (II). II (2 kg/ha) in preemergent tests killed Saccharum officinarum (sugarcane) by 0, Amaranthus (amaranth) retroflexus by 95, Poa trivialis by 100, and Echinochloa crus-galli by 100%. Herbicidal compns. containing I were reported.
IT **36721-46-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 36721-46-7 HCAPLUS
CN Propanoic acid, 2,2-dimethyl-, 3-[3,4,5,6,7,8-hexahydro-3-(1-methylpropyl)-2,4-dioxo-1(2H)-quinazolinyl]-2,2-dimethyl-3-oxopropyl ester (9CI) (CA INDEX NAME)

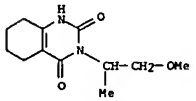
L4 ANSWER 67 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



L4 ANSWER 68 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1972:85837 HCAPLUS
DOCUMENT NUMBER: 76:85837
TITLE: Herbicidal 3-(2-alkoxy-1-methylethyl)-2,4-dioxooctahydroquinazolines
INVENTOR(S): Kiefer, Hans; Fishcher, Adolf; Koenig, Karl H.
PATENT ASSIGNEE(S): Badische Anilin- & Soda-Fabrik AG
SOURCE: Ger. Offen., 12 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2024942	A	19711202	DE 1970-2024942	19700522
ZA 7103113	A	19720223	ZA 1971-3113	19710513
NL 7106751	A	19711124	NL 1971-6751	19710517
HU 162534	P	19730328	HU 1971-BA2587	19710520
FR 2093587	A5	19720128	FR 1971-18453	19710521
AT 306429	B	19730410	AT 1971-4401	19710521
BE 767534	A1	19711124	BE 1971-103750	19710524

PRIORITY APPLN. INFO.: DE 1970-2024942 A 19700522
GI For diagram(s), see printed CA Issue.
AB The title compds. (I) with R1 = H or acyl, used as selective herbicides, were prepared from N-(2-alkoxy-1-methylethyl)-O-aminobenzamides by cyclization via 3-(2-alkoxy-1-methylethyl)-2,4-dioxotetrahydroquinazolines and hydrogenation. Thus, 489 parts isatoic anhydride reacted with H2NCHMeCH2OMe in DMF and H2O 1 hr at 80° to give 436 parts O-amino-N-(2-methoxy-1-methylethyl)benzamide, which (198 parts) was treated in PhCl with HCl(g) and then with COCl2 5-6 hr at 80° to give 158 parts 3-(2-methoxy-1-methylethyl)-2,4-dioxotetra-hydroquinazoline (II). II (83 parts) was hydrogenated in iso-PrOH over Raney Ni at 120° and 200 atm gage to give 75 parts I (R = Me, R1 = H) (III). Similarly prepared were I (R = Et, R1 = H; R = Pr, R1 = H). III (24 parts) reacted with acetoxypivaloyl chloride in Et3N and PhMe 4 hr at 80° to give 23 parts I (R = Me, R1 = AcOCH2CMe2CO). Similarly prepared were 4 addnl. 1-acyl derivs. In herbicidal tests 1 kg III/ha, e.g., was applied to the soil after sowing to kill, after 4-5 weeks, Zea mays (corn) 5, Solanum tuberosum (potato) 0, Chenopodium album 100, Poa annua 95, and Echinochloa crus-galli 90%.
IT **35239-63-5**
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study); USES (Uses)
(herbicide)
RN 35239-63-5 HCAPLUS
CN 2,4(1H,3H)-Quinazolinedione, 5,6,7,8-tetrahydro-3-(2-methoxy-1-methylethyl)- (9CI) (CA INDEX NAME)



L4 ANSWER 68 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

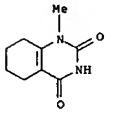
L4 ANSWER 69 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1971:510261 HCAPLUS
DOCUMENT NUMBER: 75:110261
TITLE: Ring closures from enecarbamoyl thiocyanates. Syntheses of 5,6,7,8-tetrahydro-4-thio-2,4(1H,3H)-quinazolinediones and related compounds
AUTHOR(S): Chupp, John P.
CORPORATE SOURCE: Agric. Div., Monsanto Co., St. Louis, MO, USA
SOURCE: Journal of Heterocyclic Chemistry (1971), 8(4), 565-70
CODEN: JHTCAD; ISSN: 0022-152X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 75:110261

AB Alkyl (1-cyclohexen-1-yl)carbamoyl chlorides react with thiocyanateion to form enecarbamoyl thiocyanates (I). In pyridine, I readily isomerizes to the isothiocyanate, which however is not isolated, but immediately transformed in good yields to tetrahydro-4-thio-2,4(1H,3H)-quinazolinediones (II). Various transformations of II, including conversion to tetrahydro-2,4(2H,4H)quinazolinedione, dithione, alkylation products, sodium salts and Raney Ni degradation to 4,4a,5,6,7,8,8a-octahydro-1-methyl-2(1H)quinazolinone, were carried out to investigate their chemistry and substantiate structural assignments.

IT **33738-24-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 33738-24-8 HCAPLUS
CN 2,4(1H,3H)-Quinazolinedione, 5,6,7,8-tetrahydro-1-methyl- (8CI, 9CI) (CA INDEX NAME)



L4 ANSWER 70 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1971:449125 HCAPLUS
DOCUMENT NUMBER: 75:49125
TITLE: Plant protecting uracils
INVENTOR(S): Hagemann, Hermann; Ley, Kurt
PATENT ASSIGNEE(S): Farbenfabriken Bayer A.-G.
SOURCE: Ger. Offen., 11 pp.
CODEN: GWXXEX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

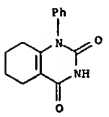
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 1959705	A	19710603	DE 1969-1959705	19691128
PRIORITY APPLN. INFO.:			DE 1969-1959705	19691128

GI For diagram(s), see printed CA Issue.

AB Title compds. (I), useful as plant protecting agents or their intermediates, were prepared by reaction of R2CH2C(R1):NR with ClCONCO (II). Thus, Me2C:NCH2Ph 73.5 reacted with II 53 in PhCl 400 g 4 hr at 30-130° with HCl evolution to give 78% I (R = CH2Ph, R1 = Me, R2 = H). Similarly prepared were 11 other I, e.g. (R-R2 given): Bu, H, Me; cyclohexyl, Et, Me; cyclohexyl, R1R2 = (CH2)4, -; Ph, R1R2 = (CH2)4, -; Me, R1R2 = (CH2)3, -.

IT **21582-83-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 21582-83-2 HCAPLUS
CN 2,4(1H,3H)-Quinazolinedione, 5,6,7,8-tetrahydro-1-phenyl- (8CI) (CA INDEX NAME)



L4 ANSWER 71 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN

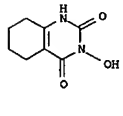
ACCESSION NUMBER: 1970:55370 HCAPLUS
DOCUMENT NUMBER: 72:55370
TITLE: Convenient route to N-3-hydroxyuracils
AUTHOR(S): Cossey, A. L.; Phillips, John N.
CORPORATE SOURCE: Div. Plant Ind., CSIRO, Canberra, Australia
SOURCE: Chemistry & Industry (London, United Kingdom) (1970), (2), 58
CODEN: CHINAG; ISSN: 0009-3068
DOCUMENT TYPE: Journal
LANGUAGE: English

GI For diagram(s), see printed CA Issue.

AB Chemical evidence is given to establish that the condensation product of A c-CH2CO2Et and HONHCONH2 in alc. NaOEt is I (R = OH, R1 = R2 = H, R3 = Me), and not the previously claimed I (R = R2 = H, R1 = OH, R3 = Me) (E. Ajello, et al., 1964). Treatment of the condensation product with p-MeC6H4SO2Cl gave an O-p-tosyl derivative, m. 204-5°, which on methylation yielded and N-methyl-O-p-tosyl derivative, m. 194-6°. Removal of the p-tosyl group by alkaline hydrolysis gave an N-methyl-N-hydroxyuracil, m. 170-1°, and subsequent reduction with Fe-AcOH gave I (R = R2 = H, R1 = R3 = Me). Similarly, hydroxyurea with Et butyrylacetate, CO(CH2CO2Me)2, and Et 2-cyclohexane-carboxylate gave, resp., I (R = OH, R1 = R2 = H, R3 = Pr), m. 178-9°; I (R = OH, R1 = R2 = H, R3 = CH2CO2Et), m. 172-3°; and I [R = OH, R1 = H, (R2R3 =) (CH2)4], m. 221-7°.

IT **26230-09-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

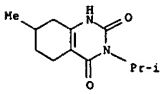
RN 26230-09-5 HCAPLUS
CN 2,4(1H,3H)-Quinazolinedione, 5,6,7,8-tetrahydro-3-hydroxy- (8CI) (CA INDEX NAME)



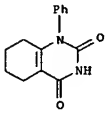
L4 ANSWER 72 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1969:115174 HCAPLUS
DOCUMENT NUMBER: 70:115174
TITLE: Herbicidal 2,4-pyrimidinediones
INVENTOR(S): Soboczenski, Edward J.
PATENT ASSIGNEE(S): du Pont de Nemours, E. I., and Co.
SOURCE: U.S., 12 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3436207	A	19690401	US 1965-434701	19650223
PRIORITY APPLN. INFO.:			US 1965-434701 A	19650223

GI For diagram(s), see printed CA Issue.
AB A variety of weeds and grasses are killed by title compds. (I), where Y is halogen, n = 3-5 and m = 0-1. A mixture of 142 g. cyclohexylurea, 170 g. Et 3-methyl-2-cyclopentanone-1-carboxylate, 10 g. 4-MeC6H4SO3H and 879 g. benzene was stirred and refluxed 8 hrs., while trapping the H2O formed. After stripping the solvent in vacuo the residue was refluxed 30 min. with 80 g. MeONa in 1 kg. absolute MeOH, the solvent stripped, the residue dissolved in H2O and the solution acidified to give 3-cyclohexyl-5,6-dihydro-7-methyl-5-cyclopenta[d]pyrimidine-2,4-(1H,3H)-dione, m. 201-3° (EtOH). The cited method and other published procedures were used to prepare a large number of I; no properties given. Preferred doses range from 0.5-2.0 lb./acre for pre-emergence use and 20-30 lb./acre for post-emergence application.
IT 22497-71-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 22497-71-8 HCAPLUS
CN 2,4(1H,3H)-Quinazolinedione, 5,6,7,8-tetrahydro-3-isopropyl-7-methyl- (8CI) (CA INDEX NAME)



L4 ANSWER 73 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1969:37768 HCAPLUS
DOCUMENT NUMBER: 70:37768
TITLE: Synthesis of 4-thiouracils
AUTHOR(S): Lamon, Robert W.
CORPORATE SOURCE: Res. Lab., Eastman Kodak Co., Rochester, NY, USA
SOURCE: Journal of Heterocyclic Chemistry (1968), 5(6), 837-44
CODEN: JHTCAD; ISSN: 0022-152X
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Ethoxycarbonyl isothiocyanate forms adducts with enamines, which on treatment with primary amines or NH3, undergo apparent "amine exchange" and cyclization to 4-thiouracil derivative. Evidence for the 4-thiouracil structure includes both spectral data and chemical transformations.
IT 21582-83-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 21582-83-2 HCAPLUS
CN 2,4(1H,3H)-Quinazolinedione, 5,6,7,8-tetrahydro-1-phenyl- (8CI) (CA INDEX NAME)



L4 ANSWER 74 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1966:456840 HCAPLUS
DOCUMENT NUMBER: 65:56840
ORIGINAL REFERENCE NO.: 65:10598h,10599a-b
TITLE: Herbicidal 3-substituted uracils
INVENTOR(S): Soboczenski, Edward J.; Luckenbaugh, Raymond W.
PATENT ASSIGNEE(S): E. I. Du Pont de Nemours & Co.
SOURCE: 17 pp.; Addn. to Brit. 968,661 (CA 61, 13326g) and Brit. 1,035,091
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

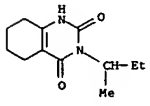
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 1035097		19660706	GB	19621207
PRIORITY APPLN. INFO.:			GB	19621207

GI For diagram(s), see printed CA Issue.
AB cf. following abstract. The parent specification claims 3-substituted uracils of I or isomeric II. In the present case the meaning ascribed to the substituent symbols is extended except insofar as the extensions are already covered by Brit. 968,666 (CA 61, 13327d). The compds. are used in conventional agricultural formulations either alone, or in admixt. with existing herbicides for the usual types of usage. Thus, 28.6 parts N-isopropylacetoacetamide and 23.6 parts iso-PrNH2 in 80 parts Et2O were kept overnight and evaporated to give 37 parts β-isopropylamino-N-isopropylcrotonamide as a viscous oil which crystallized, m. 90-3°. This (37 parts) was added with 40.8 parts Et2CO3 to a solution of 9.2 g. Na in 300 parts EtOH, the solution refluxed 22 hrs., the solvent removed in vacuo, and the residue taken up in 250 ml. water from which 29 parts 1,3-diisopropyl-6-methyluracil separated as a solid, m. 94-5°.
IT 5313-46-2, 2,4(1H,3H)-Quinazolinedione, 3-(1-ethylpropyl)-5,6,7,8-tetrahydro- (herbicide containing)
RN 5313-46-2 HCAPLUS
CN 2,4(1H,3H)-Quinazolinedione, 3-(1-ethylpropyl)-5,6,7,8-tetrahydro- (7CI, 8CI) (CA INDEX NAME)

L4 ANSWER 75 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1966:75799 HCAPLUS
DOCUMENT NUMBER: 64:75799
ORIGINAL REFERENCE NO.: 64:14196f-h
TITLE: 3-Substituted-5,6-alkylene uracil herbicides
INVENTOR(S): Soboczenski, Edward J.
PATENT ASSIGNEE(S): E. I. du Pont de Nemours & Co.
SOURCE: 15 pp.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3235360		19660215	US 1962-232311	19621022
PRIORITY APPLN. INFO.:			US	19621022

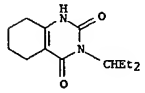
GI For diagram(s), see printed CA Issue.
AB Many weeds and grasses are selectively killed by the title compds. (I), their salts, and amine and phenol adducts. I can be prepared as described by De Stevens, et al. (CA 54, 1528g) or as follows: A mixture of 404 iso-PrNHC(O)NH2, 686 ethyl 2-cyclopentanone-1-carboxylate, 40 H3PO4, 1000 dioxane, and 879 C6H6 was stirred and refluxed 4 hrs. while the H2O formed was distilled, the solvent evaporated in vacuo, and the residue refluxed 10 min. with 2360 absolute EtOH and 248 NaOMe, the solvent evaporated, and the residue dissolved in H2O, acidified, and filtered to give 3-isopropyl-5,6-trimethyleneuracil (II), m. 222-3.5° (EtOH). Similarly prepared were the following II homologs: 3-cyclohexyl, m. 310-13° (HCONMe2); 3-allyl, m. 163.5-6.0,° and some 35 others, no properties given. Melting a mixture of 222 3-sec-butyl-5,6-tetramethyleneuracil (III) and 94 PhOH gave the 1:1 complex, m. 103-4° (cyclohexane). The p-ClC6H4OH complex of III m. 91-3° (cyclohexane). For complete destruction of vegetation 10-30 lb./acre are used; 0.5-3.0 lb. give a selective action.
IT 5313-45-1, 2,4(1H,3H)-Quinazolinedione, 3-sec-butyl-5,6,7,8-tetrahydro- (as herbicide)
RN 5313-45-1 HCAPLUS
CN 2,4(1H,3H)-Quinazolinedione, 3-sec-butyl-5,6,7,8-tetrahydro- (7CI, 8CI) (CA INDEX NAME)



L4 ANSWER 76 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1966:75798 HCAPLUS
DOCUMENT NUMBER: 64:75798
ORIGINAL REFERENCE NO.: 64:14196f
TITLE: 6-(1,2,3,4-Tetrahydro-2-thioxo-4,4,6-trimethyl-1-pyrimidinyl)-2-benzothiazolyl thiolcarbonates
INVENTOR(S): D'Amico, John J.; Tung, Ching C.
SOURCE: 2 pp.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3225049		19651221	US 1963-334040	19631227

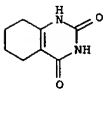
PRIORITY APPLN. INFO.: US 19631227
AB Division of U.S. 3,151,114 (CA 62, 572e). The disclosure is the same but the claims are different.
IT **5313-46-2**, 2,4(1H,3H)-Quinazolinedione, 3-(1-ethylpropyl)-5,6,7,8-tetrahydro-
(as herbicide)
RN 5313-46-2 HCAPLUS
CN 2,4(1H,3H)-Quinazolinedione, 3-(1-ethylpropyl)-5,6,7,8-tetrahydro- (7CI, 8CI) (CA INDEX NAME)



L4 ANSWER 77 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1965:3086 HCAPLUS
DOCUMENT NUMBER: 62:3086
ORIGINAL REFERENCE NO.: 62:555c-h,556a-e
TITLE: 5,6-Tetramethylenepyrimidines substituted in positions 2 and 2,4
AUTHOR(S): Budesinsky, Z.; Roubinek, F.
CORPORATE SOURCE: Vyzkumny Ustav Farm. Biochem., Prague
SOURCE: Collection of Czechoslovak Chemical Communications (1964), 29, 2341-50
CODEN: CCCCAK; ISSN: 0010-0765
DOCUMENT TYPE: Journal
LANGUAGE: German
GI For diagram(s), see printed CA Issue.
AB Condensation of CO(NH2)2 (I) with 2-ethoxalylcyclohexanone (II) gave derivs. of 2-hydroxy-5,6-tetramethylenepyrimidine-4-carboxylic acid (III). Condensation of I with 2-carbethoxycyclohexanone (IV) gave 5,6-tetramethyleneuracil (V). Condensation of CS(NH2)2 (VI) with IV gave 2-mercapto-4-hydroxy-5,6-tetramethylenepyrimidine (VII), which was desulfurized to 4-hydroxy-5,6tetramethylenepyrimidine (VIII). I (100 g.) and 140 g. II refluxed 2 hrs. with 7 ml. concentrated HCl in 500 ml. absolute EtOH gave 37.9% of a mol. compound of I with the Et ester (IIIa) of III, m. 185° (H2O), which treated with 10% NaOH gave 63% III, m. 189° (H2O). IIIa (50 g.) and 100 ml. aqueous NH3 heated 1 hr. at 100° in an autoclave gave 82% III amide (IX), m. 285° (decomposition) (H2O). IIIa (280 mg.) in 3 ml. EtOH refluxed briefly with 50 mg. N2H4.H2O gave 74.6% III hydrazide, m. 163-5° (EtOH). IX (18.9 g.) treated at 10° with NaOBr prepared from 21.7 g. Br and 24 g. NaOH in 200 ml. H2O, and the mixture heated to 75° and neutralized gave 64.5% 2-hydroxy-4-amino-5,6-tetramethylenepyrimidine (X), m. 352° (decomposition) (H2O, made alkaline with NH3). X (7 g.) refluxed with 70 ml. POCl3 and 7 ml. PhNMe2 6 hrs., the excess POCl3 distilled in vacuo, and the residue poured into H2O and neutralized with Na2CO3 gave 96% 2-chloro-4-amino-5,6-tetramethylenepyrimidine (XI), m. 182-6° (EtOH), also obtained in 94.7% yield by heating 7 g. 2,4-dichloro-5,6-tetramethylenepyrimidine (XII) with 20 ml. aqueous NH3 and 35 ml. EtOH 6 hrs. in an autoclave at 100°. A mixture of 3 g. I, 8.5 g. IV, and NaOEt prepared from 1.15 g. Na and 40 ml. EtOH refluxed 2 hrs., evaporated in vacuo, the residue dissolved in 150 ml. H2O, the solution filtered with C, and the filtrate acidified with concentrated HCl gave 36.3% V, m. 295-7° (EtOH). A suspension of 45 g. V in 200 ml. POCl3 refluxed 40 min., the mixture evaporated, and the residue poured on ice and neutralized with NH3 gave 56% XII, m. 72-3° (50% EtOH) (sublimed in vacuo at 60°). A mixture of 2 g. XII, 1.3 g. p-ClC6H4NH2 (XIII), and 10 ml. xylene refluxed 6 hrs. gave 36.5% 2-chloro-4-(p-chloroanilino)-4,6-tetramethylenepyrimidine, m. 320° (EtOH). This (3 g.) and 15 ml. 20% NH3 in EtOH, heated in an autoclave 14 hrs. at 100°, the mixture evaporated in vacuo, and the residue diluted with H2O gave 39.8% 2-amino-4-(p-chloroanilino) 5,6-tetramethylenepyrimidine, m. 174° (60% EtOH). XI (3.65 g.) and 2.5 g. XIII heated 20 min. at 120° gave 15.4% 4-amino-2-(p-chloroanilino)-5,6-tetramethylenepyrimidine, m. 312-15° (50% EtOH). A mixture of 4 g.

L4 ANSWER 77 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
XII and 5.2 g. XIII heated slowly with 0.01 ml. concd. HCl to 120°, then kept 20 min. at 165-70°, cooled, and treated with H2O alkalized with NH3 gave 63.3% 2,4-bis(p-chloroanilino)-5,6-tetramethylenepyrimidine, m. 178° (EtOH). IV (205.5 g.) and 150 g. VI in 1 l. EtOH refluxed 30 min. gave 2-cyclohexanonecarboxylic acid thioureide, which, after the addn. of EtONa prepd. from 46 g. Na and 800 ml. EtOH, refluxing 2 hrs., and dilg. with 3 l. H2O yielded 87.9% VII, m. 310°. VII (9.1 g.) in 50 ml. 2N KOH stirred 2 hrs. with 6.3 g. Me2SO4, and the mixt. neutralized with AcOH gave 56.9% 2-methylthio-4-hydroxy-5,6-tetramethylenepyrimidine, m. 220-2° (80% EtOH). A mixt. of 1.82 g. VII, NaOEt prepd. from 0.4 g. Na and 10 ml. EtOH, and 1.7 g. EtI heated 6 hrs. in a sealed tube at 100° gave 57.2% 2-ethylthio-4-hydroxy-5,6tetramethylenepyrimidine, m. 186-8° (EtOH). Treatment of 9.1 g. VII with NaOEt prepd. from 1.15 g. Na and 60 ml. EtOH and with 6 g. ClCO2Et overnight at room temp. yielded 70.9% 2-carbethoxythio-4-hydroxy-5,6-tetramethylenepyrimidine (XIIIa), m. 173-4° (HCONMe2). Similar treatment of 5 g. VII with NaOEt (from 0.63 g. Na and 30 ml. EtOH) and 3.4 g. ClCH2CO2Et gave 73.7% 2-carbethoxymethylthio-4-hydroxy-5,6-tetramethylenepyrimidine, m. 192° (EtOH), which hydrolyzed with 2N NaOH 6 hrs. at room temp. yielded 66% 2-carboxymethylthio-4-hydroxy-5,6-tetramethylenepyrimidine, m. 209° (decompn.) (50% AcOH). A suspension of 81 g. 4-hydroxy-5,6-tetramethylenepyrimidine in 400 ml. POCl3 heated slowly to boiling, refluxed 15 min., POCl3 distd. in vacuo, and the residue decompd. with ice water and neutralized with NH3 gave 88% 4-chloro-5,6-tetramethylenepyrimidine, m. 82-4° (XIV) (50% EtOH). XIV (8.4 g.), 7.6 g. VI, and 80 ml. EtOH refluxed 3 hrs., the mixt. evapd. in vacuo, and the residue in 100 ml. H2O filtered with C and acidified with HCl gave 85.7% 4-mercapto-5,6-tetramethylenepyrimidine (XV), m. 280-1° (EtOH). A mixt. of 4.5 g. XIV and an alc. soln. of 3.2 g. Me2NH heated in an autoclave 9 hrs. at 100°, evapd. in vacuo, the residue treated with 50 ml. H2O, the oil extd. with Et2O, and the ext. dried with K2CO3 and satd. with gaseous HCl gave 80% HCl salt of 4-dimethylamino-5,6-tetramethylenepyrimidine, m. 212-14° (EtOH). Treatment of 8.3 g. XV in 50 ml. N NaOH with 6.4 g. Me2SO4 gave after 2 hrs. 56.7% 4-methylthio-5,6-tetramethylenepyrimidine, m. 42° (70% MeOH). Treatment of 9 g. XIV with BuSNa (prepd. from 6.2 g. BuSH, 1.6 g. Na, and 60 ml. EtOH) gave 67.4% 4-butylthio-5,6-tetramethylenepyrimidine, b0.1 105°, n20D 1.5610. XV and ClCH2CO2Et gave 63.4% 4-carbethoxymethylthio-5,6-tetramethylenepyrimidine, m. 192° (EtOH) which, boiled briefly with 5% NaOH, yielded 57.3% 4-carboxymethylthio-5,6-tetramethylenepyrimidine, m. 175-6° (H2O). A mixt. of 40 g. VII, 400 ml. C5H5N, and 120 g. P2S5 (added portionwise) refluxed 3 hrs., the C5H5N distd., the residue treated with 2 l. H2O, the product in 4N NaOH filtered with C, and the filtrate treated with HCl gave 66.6% 2,4-dimercapto-5,6-tetramethylenepyrimidine (XVI), m. 348° (EtOH). XVI was further transformed to 71% 2,4-bis(methylthio)-5,6-tetramethylenepyrimidine, m. 78° (MeOH) (yield 71%), and to 2,4-bis(carbethoxymethylthio)-5,6-tetramethylenepyrimidine, m. 63-4° (EtOH). VII, XIIIa, and XVI were thyreostatic. VII and XVI were also analgesics.
IT **35042-48-9**, 2,4-Quinazolinediol, 5,6,7,8-tetrahydro-
(preparation of)
RN 35042-48-9 HCAPLUS
CN 2,4(1H,3H)-Quinazolinedione, 5,6,7,8-tetrahydro- (9CI) (CA INDEX NAME)

L4 ANSWER 77 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

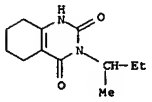


L4 ANSWER 78 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1964:476623 HCAPLUS
DOCUMENT NUMBER: 61:76623
ORIGINAL REFERENCE NO.: 61:13326g-h,13327a-e
TITLE: 3-Substituted uracils for herbicidal compositions
PATENT ASSIGNEE(S): E. I. du Pont de Nemours & Co.
SOURCE: 34 pp.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 968661		19640902	GB 1960-28141	19600815
PRIORITY APPLN. INFO.:			US	19590814

AB Compds. of the general formula I are prepared Thus, 8 parts Cl is added at <30° to a solution of 22.4 parts 3-cyclohexyl-6-methyl-2thiouracil in .apprx.100 parts HOAc and the mixture stirred 0.5 hr. at room temperature to give the 5-chloro derivative Also prepared are the following I (X, R, R1, and R2 given): O, cyclopentyl, Br, Pr; O, Br, NO2, Me (m. 170-1°); S, Am, thiocyanato, Me; S, iso-Pr, Me, Me; O, cyclopentyl, Me, Me; O, cyclohexyl, H, H; O, cyclohexyl, Me, H; O, Me, (R1R2 =) (CH2)3; O, iso-Pr, CH2OH, Me; O, iso-Pr, ClCH2, Me; O, iso-Pr, MeSCH2, Me; O, cyclopenten-2-yl, H, Me. Very ninny other examples were given with no phys. properties. Emulsifiable oils containing these compds. are useful in controlling the growth of weeds on uncultivated areas. Brit. 968,662 (Cl. A 01n), (same patentee; by Linus M. Ellis). Appl. Sept. 21, 1960; 10 pp. Addition to Brit. 968,661. A solution of 19.8 parts BuNCO in 100 parts xylene is added to a solution of 23 parts MeC(NH2):CHCO2Me in 100 parts xylene and the mixture refluxed 1 hr. to give 3-butyl-6-methylura-cil, m. 182-3° (EtOH). Also prepared is the 3-isopropyl analog, m. 186-7.5°. Other examples are given with no phys. properties. The compds. are herbicides. Brit. 968,663 (Cl. C 07cd); 12 pp. Addition to and Division of Brit. 968,661. A mixture of 28.4 parts cyclohexylurea, 28.6 parts AcCH2CO2Et, 2 parts H3PO4, 100 parts dioxane, and 88 parts C6H6 is refluxed to give 3-cyclohexyl-6-methyluracil (II), m. 233.5-5.5°. A solution of 28.8 parts II in 100 parts HOAc is treated at <30° with 8 parts Cl to give the 5-chloro derivative Similarly prepared are the following I (X = O) (R, R1, and R2 given): cyclohexyl, Br, Me; cyclopentyl, H, Me; cyclooctyl, Me, Me; cyclopentyl, (R1R2 =) (CH2)3; cyclohexyl, CH2OH, Me (m. 175-6°); cyclohexyl, MeOCH2, Me. Many other examples were given with no phys. properties. The compds. are useful in the control of weeds. Brit. 968,664; 12 pp. Addition to and Division of Brit. 968,661. A solution 18.2 parts 3-butyl-6-methyluracil in 100 parts HOAc is treated at <30° with 8 parts Cl to give 7.5 parts the 5-chloro derivative, m. 163-4° (cyclohexane-EtOAc). Similarly prepared are the following I (X = O) (R, R1, and R2 given): Bu, Br, Me, (m. 158-60°); Bu, Me, Me [m. 116.5-17° (EtOH-H2O)]; iso-amyl, Me, Me; Bu, MeO, Me; iso-Pr, Me, Me; iso-Bu, Me, Me, (K salt); iso-Pr, (R1R2 =) (CH2)3 (m. 222-3.5°); Bu, Cl, Me (Na salt); sec-Bu, (R1R2 =) (CH2)4 (Na salt). Other compds. were given with no phys. properties. The compds. are useful herbicides. Brit. 968,665; 6 pp. Addition to and Division of Brit. 968,661.
A

L4 ANSWER 78 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
soln. of 20.2 parts 3-phenyl-6-methyluracil in 100 parts HOAc is treated at <30deg; with 8 parts Cl to give the 5-chloro deriv. Similarly prepd. are the following I (X = O) (R, R1, and R2 given): Ph, Cl, Et; PhCH2, Cl, Me; Ph, Br, Me; PhCH2, Me, Me; PhCH2, Et, Et. Brit. 968,666 (Cl. C 07df), (same patentee; by Raymond W. Luckenbaugh and Edward J. Soboczenski). Appl. Aug. 15, 1960; 23 pp. Addn. to Brit. and Division of Brit. 968,661. Ketene in N is introduced at room temp. into a mixt. of 104 parts 3-butyl-5-bromo-6-methyluracil in 1000 parts Me2CO to give the 1-acetyl deriv., m. 54.5-5° (hexane). Similarly prepd. are (m.p. given): 1,3-diisopropyl-5-bromo-6methyluracil, -; 1-trichloromethylthio-3-isopropyl-5-bromo-6methyluracil, 103-5° (EtOH); 1-trichloromethylthio-3-cyclohexyl-6-methyluracil, 129-31° (EtOH-H2O). Many other examples are given with no phys. properties. The compds. are herbicides.
IT 5313-45-1, 2,4(1H,3H)-Quinazolinedione, 3-sec-butyl-5,6,7,8-tetrahydro-
(sodium derivative)
RN 5313-45-1 HCAPLUS
CN 2,4(1H,3H)-Quinazolinedione, 3-sec-butyl-5,6,7,8-tetrahydro- (7CI, 8CI) (CA INDEX NAME)



L4 ANSWER 79 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1964:82902 HCAPLUS
DOCUMENT NUMBER: 60:82902
ORIGINAL REFERENCE NO.: 60:14519c-g
TITLE: Uracils and hydrouracils
INVENTOR(S): Loux, H. M.; Luckenbaugh, R. W.; Soboczenski, E. J.
PATENT ASSIGNEE(S): E. I. du Pont de Nemours & Co.
SOURCE: 364 pp.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
PATENT INFORMATION:

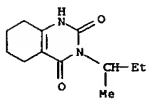
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
BE 625897		19630610	BE	
FR 1344628			FR	
NL 286546			NL	
US 3235357		19660215	US 1962-217521	19620817
US 3235361		19660215	US 1962-233952	19621029
PRIORITY APPLN. INFO.:			US	19611211

GI For diagram(s), see printed CA Issue.
AB 6-Alkyluracils were halogenated, ureas treated with alkyl 2-alkyl-3-oxoalkanoates, ureas treated with 2-cycloalkanone-1-carboxylic acid esters, and 6-alkyluracils treated with an alc. and a halogen to give I, II, III, and IV, which can be used as herbicides. Thus, 19.0 parts 3-cyclopentenyl-6-methyluracil was treated with 8.0 parts Cl to give 3-cyclopentenyl-5-chloro-6-methyluracil. Similarly prepared were I (R = H, X = O, Y = Cl, R2 = Me, R1 = sec-Bu, m. 153-5° (EtOH-H2O); I (R = H, X = O, Y = Br, R2 = Me, R1 = sec-Bu), m. 157.5-60° (EtOH-H2O); I (X = O, R = iso-Pr, R1 = iso-Pr, Y = H, R2 = Me), m. 94-5°; III(R = sec-Bu, X = Cl, X1 = Cl, Y = MeO, R1= Me), m. 144-7°; IV (R = sec-Bu, n = 3), m. 131-4°; I(X = S,R = H, R1 = Ph, Y = Br, R2 = Me), m. 230-2°. Also prepared were the following I (X = O, R = H, R2 = Me)(R1, Y, and m.p. given): iso-Pr, MeOCH2, m. 116.5-18.5°; sec-Bu, SCN, m. 157-8°. Also prepared were the following complexes (m.p. given): 1:1 3-isopropyl-5-bromo-6-methyluracil (V)-pentachlorophenol (VI), 142-3° (MeNO2); 2:1 V-PhOH, 140.5-42°; 1:1 II (R = H, R1 = sec-Bu, n = 4) (VII)-PhOH, 103-4 (cyclohexane); 222 parts VII-128 parts p-ClC6H4OH, 91-3° (cyclohexane); 1:1 HOCH2CH2NH2-V, 80-3° (MeNO2); 1:1 octylamine-V, 74-8°; 1:1 H2NCH2CH2NH2-V, 102-6°. Also prepared was the tetrabutylammonium salt (m. 164.5-7.5°) of 3-cyclohexyl-6-methyluracil. Also prepared were β-isopropylamino-N-isopropylcrotonamide, m. 90-3°, and III (R = iso-Pr, X = X1 = Cl, Y = HO, R1 = Me), m. 136.5-8.5°. Many other compds. were given without phys. consts.
IT 5313-63-3, 2,4(1H,3H)-Quinazolinedione, 3-sec-butyl-5,6,7,8-tetrahydro-, compound with phenol
(preparation of)
RN 5313-63-3 HCAPLUS
CN 2,4(1H,3H)-Quinazolinedione, 3-sec-butyl-5,6,7,8-tetrahydro-, compd. with phenol (1:1) (8CI) (CA INDEX NAME)

CM 1

CRN 5313-45-1
CMF C12 H18 N2 O2

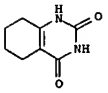
L4 ANSWER 79 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



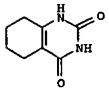
CM 2

CRN 108-95-2
CMF C6 H6 O

L4 ANSWER 80 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1962:16266 HCAPLUS
DOCUMENT NUMBER: 56:16266
ORIGINAL REFERENCE NO.: 56:3041c-d
TITLE: Condensation of N,N'-diarylthiourea with cyclohexanone. Absorption spectra of 1,3-disubstituted 2,4-dioxooctahydro-quinazoline
AUTHOR(S): Schoen, Jadwiga
CORPORATE SOURCE: Univ. Krakow, Pol.
SOURCE: Roczniki Chemii (1961), 35, 967-78
CODEN: ROCHAC; ISSN: 0035-7677
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB -Infrared and ultraviolet spectra of 1-methyl-3-phenyl- (m. 162-3°), 1-benzyl-3-phenyl- (m. 190-2°), 1,3-diphenyl-, and 1,3-bis(p-methyl-phenyl)-2,4-dioxo-1,2,3,4,5,6,7,8-octahydroquinazoline were examined. The results are discussed. They confirm the structures attributed previously to these compds. (cf. CA 50, 8660g).
IT 35042-48-9, 2,4(1H,3H)-Quinazolinedione, 5,6,7,8-tetrahydro- (derivs., spectra of)
RN 35042-48-9 HCAPLUS
CN 2,4(1H,3H)-Quinazolinedione, 5,6,7,8-tetrahydro- (9CI) (CA INDEX NAME)



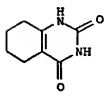
L4 ANSWER 81 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1962:16265 HCAPLUS
DOCUMENT NUMBER: 56:16265
ORIGINAL REFERENCE NO.: 56:3041a-c
TITLE: Infrared absorption spectrum and symmetry of hexaethyldisiloxane molecule
AUTHOR(S): Kirei, G. G.; Lisitsa, M. P.
SOURCE: Optika i Spektroskopiya (1961), 11, 55-60
CODEN: OPSPAM; ISSN: 0030-4034
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB -The optical d. of liquid hexaethyldisiloxane (I) was measured at 500-3050 cm.-1. Analysis and interpretation were made of the valence vibrations and deformational vibrations of C-H bonds. The comparison of the infrared spectrum of I with its Raman spectrum showed that the majority of the fundamental vibrations that appear in the absorption spectrum are absent in the Raman spectrum, and vice versa. This shows the effect of alternating restriction, indicating the presence of a symmetry center in the mol. However, this conclusion is contradicted by the fact that the SiOSi angle is not equal to 180° and that both vibrational spectra have some fundamental vibrations that coincide with each other. Thus, the selection of the symmetry group is made from the point groups C1, C3, and C2v. Previously obtained x-ray data (Skryshevskii, et al., Doklady IV Ukrain. Konf. Fiz. Khim. (Izdatel. Kharkov University) 1960, 49) showed the symmetry to be C2v.
IT 35042-48-9, 2,4(1H,3H)-Quinazolinedione, 5,6,7,8-tetrahydro- (derivs., spectra of)
RN 35042-48-9 HCAPLUS
CN 2,4(1H,3H)-Quinazolinedione, 5,6,7,8-tetrahydro- (9CI) (CA INDEX NAME)



L4 ANSWER 82 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1961:59574 HCAPLUS
DOCUMENT NUMBER: 55:59574
ORIGINAL REFERENCE NO.: 55:11445h-i
TITLE: 2,4-Diamino-5,6,7,8-tetrahydroquinazoline
INVENTOR(S): Kano, Hideo
PATENT ASSIGNEE(S): Shionogi & Co., Ltd.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 35012079		19600827	JP	

AB A mixture of 20 g. 2-oxocyclohexanecarboxylic acid and 21 g. urea was heated 3 hrs. in 100 cc. EtOH containing NaOMe (prepared from 4.5 g. Na), cooled, poured into 600 cc. H2O, and acidified with AcOH to give 8.5 g. 2,4-dihydroxy-5,6,7,8-tetrahydroquinazoline (I), m. 298-9° (EtOH). I (8.5 g.) was heated with 17 cc. POCl3 40-50 min. and the mixture poured into ice H2O to give 7 g. 2,4-dichloro-5,6,7,8-tetrahydroquinazoline (II), needles, m. 78° (dilute EtOH). II (4 g.) was heated with 20 cc. concentrated NH4OH in a stainless steel tube 8 hrs. at 150-160° to give 3 g. title compound, m. 242° (EtOH), useful as an anticancer and antibacterial substance.
IT 35042-48-9, 2,4-Quinazolinediol, 5,6,7,8-tetrahydro- (preparation of)
RN 35042-48-9 HCAPLUS
CN 2,4(1H,3H)-Quinazolinedione, 5,6,7,8-tetrahydro- (9CI) (CA INDEX NAME)



L4 ANSWER 83 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1960:56503 HCAPLUS
DOCUMENT NUMBER: 54:56503
ORIGINAL REFERENCE NO.: 54:11039h-i,11040a-g
TITLE: Pyrimidine derivatives. VI. 1,2,4-Triazolopyrimidines. 5
AUTHOR(S): Shirakawa, Kenzo
CORPORATE SOURCE: Takeda Pharm. Inds., Ltd., Osaka
SOURCE: Yakugaku Zasshi (1959), 79, 1487-92
CODEN: YKKZAJ; ISSN: 0031-6903
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB 2-Hydrazino-4,5-tetramethylene-6-hydroxypyrimidine (I) (5 g.) and 35 ml. 85% HCO2H refluxed 24 hrs., the precipitate filtered off, the filtrate concentrated in vacuo, and the residue recrystd. (H2O) gave 1.43 g. 5,6-tetramethylene-7-hydroxy-1,2,4-triazolo[4,3-a]pyrimidine (II), needles, m. 268-70°; the mother liquor from II concentrated and the residue treated with 5% HCl gave 0.24 g. 5,6-tetramethylene-7-hydroxy-1,2,4-triazolo[2,3-a]pyrimidine (III), plates, m. 271-3°. Further recrystn. (H2O) of the precipitate gave 1.28 g. 5-hydroxy-6,7-tetramethylene-1,2,4-triazolo[4,3-a]pyrimidine (IV), m. 269-71°. IV (0.1 g.) in 5 ml. 50% HCO2H refluxed 24 hrs. and the product chromatographed gave 0.02 g. III, m. 271-3°, and 0.025 g. unreacted IV, m. 269-71°. IV (0.07 g.) heated 3 min. at 270-5° and the product chromatographed gave 0.02 g. III, m. 271-3°. III (0.3 g.) and 5 ml. HBr (d. 1.49) refluxed 4.5 hrs., the product concentrated, the residue in H2O made weakly acid with NaHCO3, and treated with 0.4 g. picric acid gave 0.43 g. picrate, m. 228-30° (decomposition), of 5-amino-1,3,4-triazole (V). II (0.15 g.) and 5 ml. 80% N2H4.H2O refluxed 5 hrs., the product concentrated, the residue in dilute EtOH filtered with C, the filtrate concentrated, and the residue treated with H2O gave 4,5,6,7-tetrahydroindazolone, m. 285-8°; the mother liquor concentrated and treated with picric acid gave V picrate, m. 229-30° (decomposition). IV (0.15 g.) and 3 ml. HBr refluxed 1.5 hrs., the product concentrated, the residue in H2O treated with Na-HCO3 to pH 4, and 0.2 g. picric acid added gave 0.16 g. V picrate, m. 229-31° (decomposition). K2CO3 (7 g.) in 5 ml. H2O, 5 g. PhCH2NHC(:NNO2)NH2, and 6.5 g. Et 2-oxo-cyclohexanecarboxylate refluxed 2 hrs., H2O added, the mixture acidified with HCl, the precipitate extracted with hot C6H6, and concentrated gave 5.9 g. 2-nitroamino-3-benzyl-5,6-tetramethylene-4(3H)-pyrimidone (VI), plates, m. 180° (decomposition) (BuOH). VI (3 g.), 2 ml. 80% N2H4.H2O, and 4 ml. H2O refluxed 15 min., the product concentrated, the residue taken up in warm C6H6, and ligroine added gave 2.3 g. 2-H2NNH analog (VII) of VI, plates, m. 136-7°. VII (0.4 g.) in 4 ml. 20% HCl refluxed 50 min. gave 0.1 g. 3-benzyl-5,6-tetramethyleneuracil, needles, m. 222-3°. VII (0.7 g.) and 5 ml. HCO2H refluxed 30 min., the product concentrated, and the residue treated with H2O gave 0.2 g. 5,6-tetra-methylene-8-benzyl-1,2,4-triazolo[4,3-a]pyrimidin-7(8H)-one (VIII), m. 148-9.5° (C6H6-ligroine). V (2 g.), 3 g. 2-formylcyclohexanone, and 20 ml. EtOH refluxed 10 hrs., the product concentrated, the residue extracted with 150 ml. ligroine, and the insol. portion extracted with 25 ml. warm C6H6 gave 2.2 g. 5,6-tetramethylene-1,2,4-triazolo[2,3-a]pyrimidine (IX), columns, m. 125-7° (C6H6-ligroine); the ligroine soluble portion yielded 1.1 g. 6,7-tetramethylene-1,2,4-triazolo[2,3-a]pyrimidine (X), needles, m.

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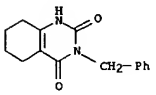
88-90°. On catalytic redn., 1 g. 7-Cl analog (m. 124-5°) of IX in 50 ml. EtOH and 0.8 g. AcOK with 0.7 g. 5% Pd-C absorbed required amt. of H in 20 min., concn. of the product, addn. of 30% NaOH, and extn. with C2H4Cl2 yielded 0.65 g. IX, m. 125-6°. I (7 g.) in 50 ml. AcOH boiled 9 hrs. and the product recrystd. (20% AcOH) gave 4.2 g. 3-methyl-5-hydroxy-6,7-tetramethylene-1,2,4-triazolo[4,3-a]pyrimidine (XI), needles, m. 265°; the H2O-sol. portion of the mother liquor from XI recrystd. (EtOCH2CH2OH) gave 0.33 g. 3-methyl-5,6-tetramethylene-7-hydroxy-1,2,4-triazolo[4,3-a]pyrimidine (XII), needles, m. 302-4°. 3-Methyl-5-amino-1,2,4-triazole (2 g.) and 3.4 g. Et 2-oxocyclohexanecarboxylate in 10 ml. AcOH boiled 10 hrs. and the residue boiled with H2O gave 2-methyl-5,6-tetramethylene-7-hydroxy-1,2,4-triazolo[2,3-a]pyrimidine (XIII), columns, m. 260-1° (H2O). IX (0.3 g.) heated 10 min. at 270-5° gave 0.16 g. XIII, m. 260-1°. 2-Hydrazino-4,5-trimethylene-6-hydroxypyrimidine (1.5 g.) in 5 ml. HC(OEt)3 and 15 ml. BuOH boiled 1 hr. and the product recrystd. (H2O) gave 5-hydroxy-6,7-trimethylene-1,2,4-triazolo[4,3-a]pyrimidine (XIV), needles, m. 227-9°, and the mother liquor yielded a small amt. of 5,6-trimethylene-7-hydroxy-1,2,4-triazolo[4,3-a]pyrimidine, plates, m. 301° (decompn.). XIV (0.1 g.) heated 5 min. at 230-5° gave 5,6-trimethylene-7-hydroxy-1,2,4-triazolo[2,3-a]pyrimidine, plates, m. 320° (decompn.).

IT **101112-63-4**, 2,4(1H,3H)-Quinazolinedione, 3-benzyl-5,6,7,8-tetrahydro-
(preparation of)

RN 101112-63-4 HCAPLUS

CN 2,4(1H,3H)-Quinazolinedione, 3-benzyl-5,6,7,8-tetrahydro- (6CI) (CA INDEX NAME)



L4 ANSWER 84 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1956:44627 HCAPLUS

DOCUMENT NUMBER: 50:44627

ORIGINAL REFERENCE NO.: 50:8660g-i,8661a

TITLE: The condensation of N,N'-diaryl derivatives of thiourea with cyclohexanone. Synthesis of new compds. of the type 1,3-diaryl-2,4-dithioxooctahydroquinazoline

AUTHOR(S): Schoen, Jadwiga

CORPORATE SOURCE: Univ. Crakow, Pol.

SOURCE: Roczniki Chemii (1955), 29, 549-66
CODEN: ROCHAC; ISSN: 0035-7677

DOCUMENT TYPE: Journal

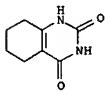
LANGUAGE: English

AB Reaction of N,N'-diaryl derivs. of thiourea with cyclohexanone (I) gave 1,3-diaryl-2,4-dithioxo-1,2,3,4,5,6,7,8-octahydroquinazoline (Ia) in addition to 9-arylamino-1,2,3,4-tetrahydroacridine. Thus, 49 g. (PhNH)2CS (II) and 20 g. I gave 3-4 g. Ia (aryl = Ph), m. 289-90° (from EtOH), which on treatment with HgO gave the 2(?)-thioxo-4(?)-oxo analog, m. 269-71° (from EtOH or dilute HOAc), and the 2,4-dioxo analog, m. 191-3° (from dilute EtOH). (p-MeC6H4NH)2CS (III) (27.55 g.) and 10 g. I gave 2.5-3 g. Ia (aryl = p-MeC6H4), m. 254-5° (from HOAc), which on HgO treatment gave the 2(?)-thioxo-4(?)-oxo analog, m. 210-11° (from 70% EtOH), and the 2,4-dioxo analog, m. 211-12.5° (from EtOH). (p-MeOC6H4NH)2CS (IV) (30 g.) and 11 g. I gave Ia (aryl = p-MeOC6H4), m. 288-9° (from C6H6), which after HgO treatment gave the 2(?)-thioxo-4(?)-oxo analog, m. 239-40° (from EtOH), and the 2,4-dioxo analog, m. 197.5-8.5° (from dilute EtOH). The same N,N'-diarylthioureas were condensed with Et tetrahydroanthranilate (V) to give 3-aryl-2-thioxo-4-oxo-1,2,3,4,5,6,7,8-octahydroquinazolines (Va). Thus, 1.7 g. V and 2.5 g. II gave 1.6 g. Va (aryl = Ph), m. 308-9° (from C6H6), which was transformed to the 2,4-dioxo analog, m. 265-6° (from C6H6). V (1.8 g.) and 3.0 g. III gave 1.5 g. Va (aryl = p-MeC6H4), m. 316-18° (from MeOH), which was transformed to the 2,4-dioxo analog, m. 304-5° (from dilute EtOH). V (1.7 g.) and 3 g. IV gave after crystallization 1 g. Va (aryl = p-MeOC6H4), m. 276-8° (from EtOH), which gave the 2,4-dioxo analog, m. 249-50° (from EtOH).

IT **35042-48-9**, 2,4(1H,3H)-Quinazolinedione, 5,6,7,8-tetrahydro-
(derivs.)

RN 35042-48-9 HCAPLUS

CN 2,4(1H,3H)-Quinazolinedione, 5,6,7,8-tetrahydro- (9CI) (CA INDEX NAME)



L4 ANSWER 85 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1954:42554 HCAPLUS

DOCUMENT NUMBER: 48:42554

ORIGINAL REFERENCE NO.: 48:7645h-i,7646a-b

TITLE: 2-Substituted 6-thia-5,6,7,8-tetrahydro-4-quinazolinol derivatives

INVENTOR(S): Rorig, Kurt

PATENT ASSIGNEE(S): G.D. Searle and Co.

DOCUMENT TYPE: Patent

LANGUAGE: Unavailable

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

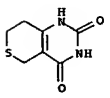
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2635101		19530414	US 1952-273140	19520223

AB Guanidine-HCl 324 and absolute alc. 2400 are mixed with a solution of NaOMe 216 in absolute alc. 2400 parts, the resulting NaCl filtered off, the Et ester 600 parts of 4-oxotetrahydrothiapyran-3-carboxylic acid (I) added to the filtrate, the precipitate filtered after 1 hr., and washed with alc., giving the monohydrate of 2-amino-6-thia-5,6,7,8-tetrahydro-4-quinazolinol (II), recrystd. from large amts. of H2O. To II 200 suspended in absolute alc. 2700 parts is added sufficient 25% anhydrous HCl in iso-PrOH to render the suspension acid and complete solution is effected by heating; the salt of II which ppts. on cooling is filtered off and recrystd. from H2O [m. 322-4° (decomposition)]; with AgNO3 in H2O is obtained a crystalline Ag salt. To a solution of Na 32 and MeOH 700 are added thiourea 43 and I 100 parts, the mixture heated in a sealed tube 5 hrs. at 100°, evaporated to dryness in vacuo, the residue dissolved in H2O, decolorized with C, filtered, and AcOH added to the filtrate, giving a precipitate of 2-mercapto-6-thia-5,6,7,8-tetrahydro-4-quinazolinol (III). Similarly, with I, urea gives upon crystallization from EtOCH2CH2OH 6-thia-5,6,7,8-tetrahydro-2,4-quinazolinediol (IV), and MeC(NH)NH2.HCl with I gives 2-methyl-6-thia-5,6,7,8-tetrahydro-4-quinazolinol (V). The Me ester of I with HNC(SMe)NH2 sulfate gives the 2-MeS derivative (VI), and PhC(:NH)NH2.HCl gives the 2-Ph (VII) derivative The compds. are useful as coronary dilators, diuretics, and internal parasiticides.

IT **857956-61-7**, 5H-Thiapyrano[4,3-d]pyrimidine-2,4-diol, 7,8-dihydro-
(preparation of)

RN 857956-61-7 HCAPLUS

CN 5H-Thiapyrano[4,3-d]pyrimidine-2,4-diol, 7,8-dihydro- (5CI) (CA INDEX NAME)

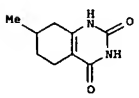


L4 ANSWER 85 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

L4 ANSWER 86 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1948:27431 HCAPLUS
DOCUMENT NUMBER: 42:27431
ORIGINAL REFERENCE NO.: 42:5854d-i,5855a-b
TITLE: Condensed thiouracils
AUTHOR(S): Polonovski, Michel; Libermann, D.
SOURCE: Bulletin de la Societe Chimique de France (1947) 1073-5
CODEN: BSCFAS; ISSN: 0037-8968
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
GI For diagram(s), see printed CA Issue.
AB The condensation of thiourea (I) with β-keto esters (II) in EtOH with NaOEt to form thiouracil derivs. (III) goes poorly when II is cyclic; II in alkaline solution undergoes ring opening and conversion to dicarboxylic acids.

A 2-stage reaction gives better yields: (1) I and II at 140-60°/20-40 mm. form the ureide intermediate with elimination of EtOH; (2) cyclization to III is carried out in alc. KOH. A trace of H3BO3 catalyzes reaction (1); excess I is used. Et 2-oxocyclopentanecarboxylate (IV) and 1.2 moles I, heated at 130-40° until no more EtOH distilled and refluxed in 1 l. N alc. KOH 2 hrs., gave 30-40% 5,6-trimethylenethiouracil, m. 340° (decomposition), yellow crystals from EtOH (cf. C.A. 40, 1454.6). IV was obtained in 70% yield from Et adipate in C6H6 and NaOEt (free of EtOH), after 24 hrs. at 15-30° and 6 hrs. at 78°. H2NC(SEt): NH in H2O and IV in Et2O were shaken vigorously with the gradual addition of 1 mole 10% aqueous Na2CO3 to form 2-(ethylmercapto)-4-hydroxy-5,6-trimethylenepyrimidine, m. 235° (from EtOH), shows blue fluorescence in ultraviolet light; heating with HCl gave EtSH and 5,6-trimethyleneuracil. 5,6-Tetramethylenethiouracil (V), obtained from Et 2-oxocyclohexanecarboxylate and I at 155-60°, m. 310° (decomposition), slightly yellow prisms; classical condensation with NaOEt instead of reactions (1) and (2) gave a completely white product. 5,6-Tetramethyleneuracil, obtained from 3 g. V and 3 g. ClCH2CO2H in 25 cc. H2O at 100° 2 hrs., m. 305° (from EtOH); mixed m.p. with V, 275°. 5,6-Indonethiouracil (VI), from 10 g. I, 20 g. of the Na derivative of Et 1,3-diketo-2-indancarboxylate (VII) (cf. Wislicenus, Ann. 246, 347(1888)), and 2.3 g. Na in boiling EtOH 6 hrs., m. 360° (decomposition, on Maquenne block), orange crystals with 3 H2O from H2O, violet color at 104°, orange again at 315°, insol. in most. organic solvents. VII, very unstable at high temps., when heated with I decompose and condenses to VIII, m. 207° (from dioxane). The phenylhydrazone derivative (prepared from an aqueous solution of VI), dissolved in boiling EtOH, cooled, and treated with a trace of Na and heated, forms a dark solution After addition of H2O, the Et2O-soluble product in concentrated H2SO4 and 1 drop of K2Cr2O7 solution gives an emerald-green to blue color, characteristic of pyrazoline. 5,6-Bornylenethiouracil (IX), formed very slowly in poor yield from I and Et 3-camphorcarboxylate in the presence of NaOEt, m. 71° (from ligroin).
IT **35042-48-9**, 2,4(1H,3H)-Quinazolinedione, 5,6,7,8-tetrahydro- (preparation of)
RN 35042-48-9 HCAPLUS
CN 2,4(1H,3H)-Quinazolinedione, 5,6,7,8-tetrahydro- (9CI) (CA INDEX NAME)

L4 ANSWER 87 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1909:11603 HCAPLUS
DOCUMENT NUMBER: 3:11603
ORIGINAL REFERENCE NO.: 3:2141a-f
TITLE: Behavior of Ammonia and Amines toward Tetrahydrosalicylic Esters
AUTHOR(S): Kotz, A.; Merkel, B.
CORPORATE SOURCE: Gottingen
SOURCE: Journal fuer Praktische Chemie (Leipzig) (1909), 79, 102-35
CODEN: JPCEAO; ISSN: 0021-8383
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
GI For diagram(s), see printed CA Issue.
AB Methyltetrahydro-anthranilic ester and PhNH2, at 200°, yielded alc. and a cyclic compound (I), long transparent needles, m. 161°. Heated at 280°, a bimolecular cyclic compound (II), yellow-white crystals, m. 300°. When ethyl-4-methyl-2-hexanone-1-carboxylate was heated with PhNH2, it yielded the corresponding dianilide (III), m. 130°. With benzylamine, the monobenzylamide (IV), m. 61°. With pyridine, the monopyridide, C15H25NO2, m. 123°. With urea and EtONa, methyltetrahydrobenzoyleneurea (V). With benzamidine hydrochloride, methylphenylketotetradihydroquinazoline (VI), m. 227°. With piperazine, ethylpiperazinedimethylhexenecarboxylate (VII), m. 216°. When ethyl 2-cyclohexanone-1-carboxylate was heated with PhNH2, it yielded the monoanilide, C15H19NO2, m. 29°. With piperazine, at 250°, the cyclic compound (VIII), m. 280°.
IT **104829-77-8**, 2,4(1,3)-Quinazolinedione, 5,6,7,8-tetrahydro-7-methyl- (preparation of)
RN 104829-77-8 HCAPLUS
CN 2,4(1H,3H)-Quinazolinedione, 5,6,7,8-tetrahydro-7-methyl- (9CI) (CA INDEX NAME)



L4 ANSWER 86 OF 87 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)